

Technical Report No. 32-660

*The JPL Thermochemistry and Normal Shock
Computer Program*

T. E. Horton

FACILITY FORM 602

N 65 15219
(ACCESSION NUMBER)
42
(PAGES)
Cl 60257
(NASA CR OR TMX OR AD NUMBER)

1
(THRU)
08
(CODE)
(CATEGORY)



JET PROPULSION LABORATORY
CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CALIFORNIA

November 1, 1964

GPO PRICE \$ _____

OTS PRICE(S) \$ _____

Hard copy (HC) 2.00

Microfiche (MF) .50

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Prepared Under Contract No. NAS 7-100
National Aeronautics & Space Administration

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ABSTRACT

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A computer program capable of calculating chemical equilibrium properties associated with traveling, standing, and reflected normal shocks has been developed. The initial gas mixture, temperature, and pressure can be varied with ease. The program can also be used to generate Mollier thermodynamic data and chemical composition at selected temperatures and densities. Both dissociation and ionization effects are considered in the temperature range of 2000 to 20,000° K. At the present time, the program is set up to consider mixtures (containing up to 36 species) which are composed of carbon, nitrogen, oxygen, and argon.

author

I. INTRODUCTION

Current studies of the feasibility of planetary entry at high velocities have created a need for rapid solution techniques of aerothermodynamic problems involving the high-temperature properties of gas mixtures. Although most problems in the field of aerothermodynamics are characterized by large force, chemical composition, and temperature gradients and thus by nonequilibrium phenomena, there are many processes of interest to the aerothermodynamist for which either the gradients disappear or the reaction rates are sufficiently fast so that the assumption of chemical equilibrium is rational. This Report is confined to the problem of supplying thermodynamic properties and chemical composition of multi-component, high temperature, real gas mixtures which satisfy the conditions of chemical equilibrium.

Several numerical techniques have been adapted to the high-speed digital computer for the calculation of the chemical equilibrium composition of gas mixtures. A survey of these techniques is given in Ref. 1. Several workers, including Gilmore (Ref. 2), Hilsenrath (Ref. 3), and Fenner (Ref. 4), have used these computer techniques to generate thermodynamic data in the form of Mollier diagrams for air-like mixtures. These thermodynamic data have been used in investigating normal shock, flow field, communication-blackout, convective heat transfer, and radiative heat transfer problems. While the procedure of generating thermodynamic data and using it for a separate calculation of normal shock parameters is adequate for air calculations, the investigation of these parameters for proposed planetary atmospheres

calls for a completely mechanized solution scheme because of the many possible gas mixture combinations.

The JPL Normal Shock and Chemical Equilibrium Program is such a scheme which is programmed in Fortran II for use on an IBM 7090 or 7094 computer. The program calculates chemical equilibrium properties associated with traveling, standing, and reflected normal shocks. The initial gas mixture, temperature, and pressure can be varied with ease. The program can handle mixtures of gases in which both dissociation and ionization are important. The capacity of the program is limited to

36 different compounds which are combinations of up to 6 different elements. The output is a complete thermodynamic and chemical description of the gas which satisfies the Hugoniot equation for the important normal shock cases which are useful in both shock tube experimentation and free-flight entry calculations.

The program can also be used to generate Mollier thermodynamic data at selected temperatures and densities if this option is desired. A mathematical statement of the criterion for chemical equilibrium is given prior to further discussion of the details of the computer program.

II. CHEMICAL EQUILIBRIUM

The bases for determining the chemical equilibrium composition of a system are the principle of conservation of mass of elemental species and the second law of thermodynamics. For the mass of the elements to be conserved the total mass of each element in the mixture (which is equal to the sum of the masses of elements in combined form as molecules and ions plus the mass in uncombined atomic form) must be a constant. From the second law of thermodynamics the increase in entropy principle follows. This principle, as shown by Zermansky (Ref. 5), applied to a constant mass system in mechanical and thermal equilibrium at a particular temperature and pressure, requires the chemical composition of the system to be such that the Gibbs free energy is a minimum.

To translate these verbalisms into mathematical expressions, the following conventions are introduced. For a mixture composed of m number of chemical elements which combine to form s number of compounds, the compounds will be identified by the numbers 1, 2, 3, ..., s and the elements by the numbers $s+1, s+2, s+3, \dots, s+m$. Further, let the symbols $X^{(s+1)}, X^{(s+2)}, X^{(s+3)}, \dots, X^{(s+m)}$ be used to represent the usual symbols for the chemical elements so that the compounds and ions of the mixture can be written as

$$Y^{(p)} = X_{\alpha_{p,s+1}}^{(s+1)} X_{\alpha_{p,s+2}}^{(s+2)} X_{\alpha_{p,s+3}}^{(s+3)} \cdots X_{\alpha_{p,s+m}}^{(s+m)}$$

where $1 \leq p \leq s$. The α_{ij} indicates the number of atoms of the j th numbered element in the i th numbered compound or ion. The α_{ij} 's come from the set of positive and negative real integers which include zero.

The assumption is made that the long-range interactions between particles of the gas mixture are negligible so that the collision times are small compared to times between collisions. This allows the behavior of the individual constituents of the mixture to be described by the ideal gas relations

$$P_i = \frac{N_i}{V} RT \quad (1)$$

and

$$C_{v,i} = f(T)$$

and the behavior of the mixture of gases to be described as an ideal solution with the chemical potential of each constituent taking the form

$$\mu_i = f_i^\circ + RT \ln P_i \quad (2)$$

Thus, the free energy of the mixture takes the form

$$\frac{F}{RT} = \sum_{i=1}^{s+m} N_i \left(\frac{f_i^\circ}{RT} + \ln P_i + \ln \frac{N_i}{N} \right) \quad (3)$$

where the terms are defined by

$$N = \sum_{i=1}^{s+m} N_i$$

and

$$\frac{f_i^\circ}{RT} = \frac{h_{o,i}^\circ}{RT} - \int \int \frac{C_{P,i}}{R} dT \frac{dT}{T^2}$$

The f_i° is a function of temperature only and is the partial molal free energy of the i th constituent evaluated at a pressure of 1 atm and the temperature in question. The $h_{o,i}^\circ$ is the molal heat of formation of the i th constituent at 0° Kelvin and 1 atm.

The condition which is imposed on the equilibrium composition by the requirement that the free energy be a minimum at a particular value of temperature and pressure is obtained by differentiating equation (3) so that

$$d \frac{F}{RT} = 0 = \sum_{i=1}^{s+m} \left[\frac{f_i^\circ}{RT} + \ln P + \ln \frac{N_i}{N} \right] dN_i \quad (4)$$

The constraint of conservation of mass of chemical elements requires that

$$0 = dN_j + \sum_{i=1}^s \alpha_{ij} dN_i \quad (5)$$

where $j = s+1, s+2, \dots, s+m$. By combining Eqs. (4) and (5) so that the $dN_{s+1}, dN_{s+2}, \dots, dN_{s+m}$ are eliminated, the following expression results:

$$0 = \sum_{i=1}^s dN_i \left[\left(\frac{f_i^\circ}{RT} + \ln P + \ln \frac{N_i}{N} \right) - \sum_{j=s+1}^{s+m} \alpha_{ij} \left(\frac{f_j^\circ}{RT} + \ln P + \ln \frac{N_j}{N} \right) \right] \quad (6)$$

As the variations in the concentrations ($dN_1, dN_2, dN_3, \dots, dN_s$) are independent, the above expression is zero only if

$$\frac{f_i^\circ}{RT} + \ln P + \ln \frac{N_i}{N} = \sum_{j=s+1}^{s+m} \alpha_{ij} \left(\frac{f_j^\circ}{RT} + \ln P + \ln \frac{N_j}{N} \right) \quad (7)$$

with $i = 1, 2, 3, \dots, s$. Rearranging this expression using

$$P \frac{N_i}{N} = \frac{N_i}{V} RT = n_i RT$$

gives

$$\frac{n_i}{\prod_{j=s+1}^{s+m} n_j^{\alpha_{ij}}} = (K_i) (RT)^{-1 + \sum_{j=s+1}^{s+m} \alpha_{ij}} \quad (8)$$

with $i = 1, 2, 3, \dots, s$ where

$$\ln K_i = - \frac{f_i^\circ}{RT} + \sum_{j=s+1}^{s+m} \alpha_{ij} \frac{f_j^\circ}{RT}$$

Equation (8) is the familiar "equation of mass action." The other constraints on the concentrations supplied by the conservation of mass of chemical elements require that

$$n_j + \sum_{i=1}^s n_i \alpha_{ij} = B_j \rho / \rho_0 \quad (9)$$

for $j = s+1, s+2, s+3, \dots, s+m$, where

B_j = concentration of the j th element at standard temperature and pressure and

ρ_0 = density of the mixture at standard temperature and pressure.

Equation (9) is frequently referred to as the "equation of mass balance." The solution of the s mass action equations and the m mass balance equations for a given temperature, density, and concentration of elements at standard conditions is a set of $s+m$ concentrations which satisfy the criterion of chemical equilibrium.

After the equilibrium concentrations have been determined, the thermodynamic properties of the gaseous mixture are calculated by the following relations:

$$n = \sum_{i=1}^{s+m} n_i$$

$$\rho = \sum_{i=1}^{s+m} n_i M_i$$

$$H = \frac{\sum_{i=1}^{s+m} n_i h_i^\circ}{\rho}$$

$$Z = \frac{\frac{P}{\rho RT}}{\frac{P_0}{\rho_0 RT_0}} = \frac{M_0}{M} \quad (10)$$

$$\frac{SM_0}{R} = \frac{M_0}{\rho} \sum_{i=1}^{s+m} n_i \left(\frac{h_i^\circ - f_i^\circ}{RT} - \ln P - \ln \frac{n_i}{n} \right)$$

The quantities which appear above are defined as:

- h_i° specific enthalpy of the i th constituent at one atmosphere.
- M_i molecular weight. Whether in lb/lb-mole or g/g-mole, the values are identical.
- M_0 molecular weight of mixture at STP.
- n total concentration of mixture, mole/l.

n_i concentration of the i th constituent.

R universal gas constant = 1.9860 Btu/ $^{\circ}$ R-lb-mole
= 1.98726 cal/ $^{\circ}$ Kg-mole.

S entropy.

$\frac{SM_0}{R}$ dimensionless entropy.

T temperature.

T_0 standard temperature = 273.15 $^{\circ}$ K.

ρ mass density.

III. NORMAL SHOCK PROBLEM

From the aerothermodynamic point of view, one of the most important yet simplest applications of the chemical equilibrium data described above is the normal shock problem. The equations governing the variation of properties through a normal shock, when the coordinate system is chosen so the flow is steady and one dimensional, and when the effects of body forces, diffusion, and radiative transfer are negligible, are:

continuity

$$\frac{d}{dx} (\rho U) = 0, \quad (11)$$

linear momentum

$$\rho U \frac{dU}{dx} + \frac{dP}{dx} = \frac{1}{2} \frac{d}{dx} \left(\eta \frac{dU}{dx} \right), \quad (12)$$

and energy

$$\rho U \frac{dE}{dx} + P \frac{dU}{dx} = \frac{d}{dx} \left(K \frac{dT}{dx} \right) + \frac{1}{2} \eta \left(\frac{dU}{dx} \right)^2 \quad (13)$$

Integration of these equations with respect to x yields

$$\rho U = C_1 \quad (14)$$

$$\rho U^2 + P = \frac{1}{2} \eta \frac{dU}{dx} + C_2 \quad (15)$$

$$\rho U \left(H + \frac{U^2}{2} \right) = \left(K \frac{dT}{dx} + \frac{1}{2} \eta U \frac{dU}{dx} \right) + C_3 \quad (16)$$

where C_1 , C_2 , and C_3 are constants. If these equations are applied across a normal shock, and if either: 1) the fluid is assumed to be inviscid ($\eta = 0$) and nonheat-conducting ($K = 0$), or 2) the fluid is assumed to be in thermodynamic equilibrium (i.e., the gradients are zero), then the equations reduce to the form

$$\rho_A U_A = \rho_B U_B \quad (17)$$

$$\rho_A U_A^2 + P_A = \rho_B U_B^2 + P_B \quad (18)$$

$$H_A + \frac{U_A^2}{2} = H_B + \frac{U_B^2}{2} \quad (19)$$

Therefore, Eqs. (17), (18), and (19) relate the thermodynamic properties and velocities in the up-stream and down-stream equilibrium regions of the flow field associated with a standing normal shock as shown in Fig. 1.

Three special applications of Eqs. (17), (18), and (19) to the equilibrium regions of shock flows are 1) the moving shock problem, 2) the standing shock problem, and 3) the reflected shock problem.

The free-flight or moving shock problem is of interest for determining the velocities and thermodynamic properties behind the normal portion of the bow shock asso-

ciated with a high velocity blunt body. The free-flight problem is equivalent to the moving shock problem in a shock tube. Physically, the problem is the determination of the properties behind a shock which is propagating

in quiescent gas at a specified velocity. Mathematically, the problem is to satisfy the Hugoniot equation,

$$H_B - H_A = \frac{1}{2} (P_B - P_A) \left(\frac{1}{\rho_A} + \frac{1}{\rho_B} \right), \quad (20)$$

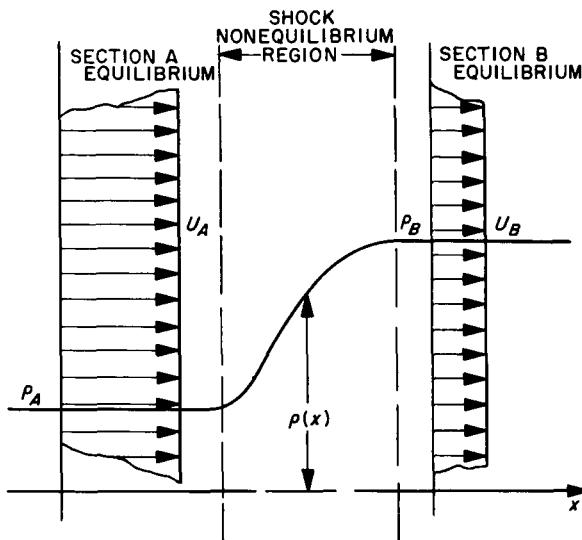
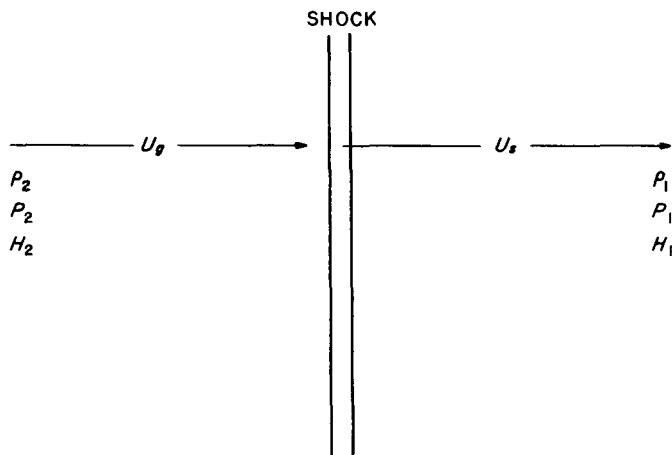


Fig. 1. Flow field associated with a normal shock



EQUATIONS TO BE SATISFIED:

$$H_2 - H_1 = \frac{1}{2} (P_2 - P_1) \left(\frac{1}{P_1} + \frac{1}{P_2} \right) \quad (21)$$

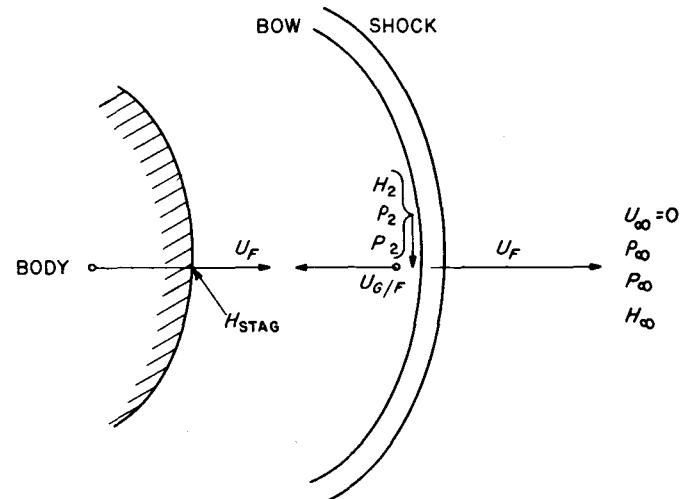
$$U_s = \sqrt{\frac{P_2}{P_1}} \left(\frac{P_2 - P_1}{P_2 + P_1} \right) = \text{SHOCK VELOCITY}, \quad (22)$$

$$U_g = U_s \left(1 - \frac{P_1}{P_2} \right) = \text{GAS VELOCITY} \quad (23)$$

Fig. 2. Moving normal shock

which is obtained from a suitable manipulation of Eqs. (17), (18), and (19). The initial properties H_A , P_A , and ρ_A are known, and the chemical equilibrium computation yields relations for H_B (ρ_B , T_B) and P_B (ρ_B , T_B). Thus, by selecting one property in region (B), the other properties are determined by Eq. (20). The Hugoniot equation and the auxiliary equations are shown in Figs. 2 and 3 with subscripts appropriate to the freeflight and moving shock problems.

The standing shock case involves the flow of the high enthalpy gas behind a moving shock over a stationary blunt body. Physically, the problem is the determination of the conditions in the equilibrium region immediately behind the bow shock associated with the body. The



EQUATIONS TO BE SATISFIED:

$$H_2 - H_\infty = \frac{1}{2} (P_2 - P_\infty) \left(\frac{1}{P_\infty} + \frac{1}{P_2} \right) \quad (24)$$

$$U_F = \sqrt{\frac{P_2}{P_\infty}} \left(\frac{P_2 - P_\infty}{P_2 + P_\infty} \right) = \text{FLIGHT VELOCITY} \quad (25)$$

$$U_{G/F} = \sqrt{\frac{P_\infty}{P_2}} \left(\frac{P_2 - P_\infty}{P_2 + P_\infty} \right) = \text{VELOCITY OF GAS RELATIVE TO THE BODY} \quad (26)$$

$$H_{STAG} = H_2 + \frac{1}{2} U_{G/F}^2 = \text{STAGNATION ENTHALPY}$$

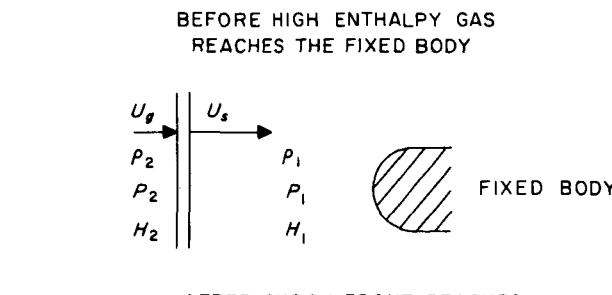
Fig. 3. Free-flight bow shock

important thermodynamic properties and velocities are indicated in Fig. 4. Also shown in this figure are the appropriate forms of Eqs. (17), (18), and (19) which for known U_g , ρ_2 , H_2 , P_2 and the implicit chemical equilibrium property relations $H_3(T_3, \rho_3)$ and $P_3(T_3, \rho_3)$ allow the velocities and state of the gas behind the standing shock to be determined. The results of this type of calculation are useful in shock tube simulation of entry conditions.

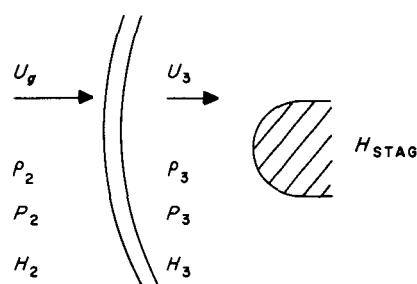
The third problem of interest, the reflected shock case, involves the stagnation of the high enthalpy gas of a moving shock by an immovable plane surface. The fluid comes to rest at the surface, and a reflected shock

propagates into the gas flowing toward the surface. The thermodynamic properties and velocities are defined in Fig. 5 along with the equations to be satisfied. Other than a slightly different form of the equations, the mathematical problem here is equivalent to the standing shock case described earlier. The results of this type of calculation are useful in interpreting experiments performed at the end of a shock tube.

Before considering the numerical techniques used to satisfy the chemical equilibrium and normal shock equations given above, it is important to reemphasize that these equations approximate shock tube and free-flight conditions only where the gas is in chemical equilibrium and the effect of wall shear and heat transfer are negligible.



AFTER SHOCK FRONT REACHES THE FIXED BODY



EQUATIONS TO BE SATISFIED

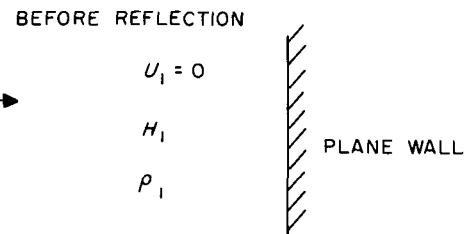
$$H_3 = H_2 + \frac{U_g^2}{2} \left[1 - \left(\rho_2 / \rho_3 \right)^2 \right] \quad (27)$$

$$\rho_3 = \rho_2 + \rho_2 U_g^2 \left[1 - \rho_2 / \rho_3 \right] \quad (28)$$

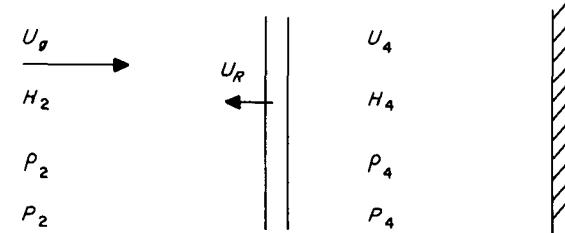
$$U_3 = \left(\rho_2 / \rho_3 \right) U_g \quad (29)$$

$$H_{STAG} = H_3 + \frac{U_3^2}{2} \quad (30)$$

Fig. 4. Standing shock



AFTER REFLECTION



EQUATIONS TO BE SATISFIED:

$$H_4 = H_2 + \frac{U_g^2}{2} \left(\frac{\rho_4 / \rho_2 + 1}{\rho_4 / \rho_2 - 1} \right) \quad (31)$$

$$\rho_4 = \rho_2 + \rho_2 U_g^2 \left(\frac{\rho_4 / \rho_2}{\rho_4 / \rho_2 - 1} \right) \quad (32)$$

$$U_R = \frac{U_g}{\rho_4 / \rho_2 - 1} = \text{REFLECTED SHOCK VELOCITY} \quad (33)$$

Fig. 5. Reflected shock

IV. NUMERICAL PROCEDURE

A. Chemical Equilibrium

To obtain the $s+m$ constituents of a gaseous mixture in chemical equilibrium requires the simultaneous solution of the m mass balance equations and the s nonlinear mass action equations. The Newton-Raphson method is well suited for solving such a system of simultaneous algebraic equations with a high speed digital computer. The Newton-Raphson method applied to the present problem allows a solution to be obtained by an iterative procedure which involves solving a linearized form of Eqs. (8) and (9). The method assumes that a point defined by a set of concentrations which nearly satisfy the mass action and mass balance conditions is known. By expanding the mass action and mass balance equations in a Taylor series about the near solution point and neglecting terms of the series which contain derivatives higher than the first order, a system of linear equations is obtained which approximate the mass action and mass balance equations. The solution of the linear system of equations results in a new set of concentrations which are nearer the actual solution to the mass action and the mass balance equations. Clearly, by repeating this procedure, a better set of concentrations can be found so that by iterating enough times a solution with any desired accuracy can be found. With a high-speed digital computer this procedure is quite simple, fast, and accurate.

The linearized form of the mass action (Eq. 8) and mass balance (Eq. 9), obtained from the series expansion with the temperature, density, and initial molar concentration constant, are of the following form:

1. Mass action

$$(Z_k)_{p+1} - \sum_{j=s+1}^{s+m} a_{kj} (Z_j)_{p+1} + (D_k)_p = 0 \quad (33)$$

where

$$k = 1, 2, 3, \dots, s$$

$(\)_p$ = indicates value from the p th iteration

$$(D_k)_p = \ln (n_k)_p + \ln RT + \frac{f_k^\circ}{RT}$$

$$- \sum_{j=s+1}^{s+m} a_{kj} \left[\ln (n_j)_p + \ln RT + \frac{f_j^\circ}{RT} \right]$$

2. Mass balance

$$(n_j)_p (Z_j)_{p+1} + \sum_{k=1}^s a_{kj} (n_k)_p (Z_k)_{p+1} + (D_j)_p = 0 \quad (34)$$

where

$$j = s+1, s+2, s+3, \dots, s+m$$

and

$$(D_j)_p = (n_j)_p + \sum_{k=1}^s a_{kj} (n_k)_p - \frac{B_j \rho}{\rho_0}$$

In the above expressions,

$$(Z_i)_{p+1} = \ln (n_i)_{p+1} - \ln (n_i)_p$$

The use of the natural logarithm of the concentration as the variable in the series expansion was suggested in Ref. 6 and was found to give good results.

This linear system of $s+m$ equations can be simplified to m equations by using Eq. (33) to eliminate $Z_1, Z_2, Z_3, \dots, Z_s$ from Eq. (34). The result of this substitution is a system of m linear equations of the form:

$$\sum_{j=1}^m (Y_{ij})_p (Z_{s+i})_{p+1} = (C_i)_p \quad (35)$$

where $i = 1, 2, 3, \dots, m$. The quantities Y_{ij} and C_i are given by

$$(Y_{ij})_p = \delta_{ij} (n_{s+i})_p + \sum_{k=1}^s (n_k)_p (a_{k,s+i}) (a_{k,s+i})$$

$$\delta_{ij} = 0 \quad \text{for } i \neq j$$

$$\delta_{ij} = 1 \quad \text{for } i = j$$

and

$$(C_i)_p = - \left[(D_{s+i})_p - \sum_{k=1}^s (n_k)_p (D_k)_p (a_{k,s+i}) \right]$$

To use Eq. (35) in obtaining a solution to Eqs. (8) and (9), the following procedure is used:

1. Using initial guesses, $(n_1)_0, (n_2)_0, (n_3)_0, \dots, (n_{s+m})_0$, for the concentrations at a selected temperature, density, and concentration of chemical elements at

standard conditions, the coefficients $(D_i)_0$ and $(Y_{ij})_0$ are evaluated.

2. A solution to the system of Eq. (35) is found using the Crout method (Ref. 7). The solution $(Z_{s+1})_1$, $(Z_{s+2})_1$, $(Z_{s+3})_1$, ..., $(Z_{s+m})_1$ yields values for $(n_{s+1})_1$, $(n_{s+2})_1$, $(n_{s+3})_1$, ..., $(n_{s+m})_1$,
3. The $(n_1)_1$, $(n_2)_1$, $(n_3)_1$, ..., $(n_s)_1$ are evaluated using Eq. (33).
4. The new values of the concentration $(n_i)_1$ with $i = 1, 2, 3, \dots, s+m$ replace the initial guesses, and the above procedure is repeated k times until

$$1 - \left| \frac{(n)_k}{(n)_{k+1}} \right| < 10^{-6}$$

and

$$1 - \left| \frac{(\rho)_k}{(\rho)_{k+1}} \right| < 10^{-6}$$

and

$$1 - \left| \frac{(\bar{H})_k}{(\bar{H})_{k+1}} \right| < 10^{-6}$$

where

$(\quad)_k$ = value from the $(k+1)$ iteration

n = total concentration

ρ = density of mixture

\bar{H} = enthalpy per unit volume

This convergence criterion has been found to result in a set of concentrations $(n_1)_{k+1}$, $(n_2)_{k+1}$, $(n_3)_{k+1}$, ..., $(n_{s+m})_{k+1}$ which agree with $(n_1)_k$, $(n_2)_k$, $(n_3)_k$, ..., $(n_{s+m})_k$ to at least three significant figures.

B. Moving and Free-Flight Normal Shock Case

The moving shock problem, as discussed earlier, consists of finding a thermodynamic state defined by T_2 and ρ_2 which satisfies the Hugoniot equation for specified initial conditions. The initial conditions are specified by the pressure, temperature, and concentrations. To find a final state which satisfies the Hugoniot equation, a final

temperature T_2 is specified and the value of ρ_2 is varied until values of p_2 and H_2 are found which satisfy the Hugoniot equations. After the properties which satisfy the Hugoniot equations are found, the Eqs. (22), (23), (25), and (26) are evaluated.

The systematic procedure for finding the correct value of ρ_2 is based on a Newton-Raphson iteration scheme in which the Hugoniot equation

$$\begin{aligned} F(v_2, T_2) &= [H_2(v_2, T_2) - H_1] \\ &\quad - \frac{1}{2} [P_2(v_2, T_2) - P_1] \left[\frac{1}{\rho_1} + v_2 \right] \end{aligned} \quad (36)$$

is expanded in v_2 at some near solution point with T_2 held constant. The resulting iteration relation for the n th iteration is

$$(v_2)_{n+1} = \left(\frac{1}{\rho_2} \right)_{n+1} = \left(\frac{1}{\rho_2} \right)_n - \frac{F((v_2)_n, T_2)}{\left(\frac{\partial F}{\partial v_2} \right)_{T_2}} \quad (37)$$

where the partial derivative is evaluated by

$$\left(\frac{\partial F}{\partial v_2} \right)_{T_2} = \frac{F((v_2)_n + (\Delta v_2)_n, T_2) - F((v_2)_n, T_2)}{\Delta v_2}$$

with

$$(\Delta v_2)_n = 10^{-6} (v_2)_n$$

The Hugoniot equation is considered satisfied after n iterations if:

$$\left| \frac{(1/\rho_2)_{n+1} - (1/\rho_2)_n}{(1/\rho_2)_n} \right| \leq 10^{-3}$$

C. Reflected and Standing Normal Shock Cases

The procedures followed for the reflected shock case and the standing shock case are similar. Therefore, only the reflected shock case will be discussed below.

The problem in the reflected shock case is to find a T_4 and ρ_4 associated with values of H_4 and ρ_4 which satisfy

Eqs. (31) and (32). The values of H_2 , p_2 , ρ_2 , and U_g are known from the moving normal shock solution.

The solution technique is based upon a series expansion of the thermodynamic properties H and p about some point (T_a, ρ_a) which is near (T_4, ρ_4) . The truncated series are of the form

$$H = H_a + \frac{\partial H}{\partial \rho} \Big|_a \delta\rho + \frac{\partial H}{\partial T} \Big|_a \delta T \quad (38)$$

$$P = P_a + \frac{\partial P}{\partial \rho} \Big|_a \delta\rho + \frac{\partial P}{\partial T} \Big|_a \delta T \quad (39)$$

with

$$\delta\rho = \rho - \rho_a$$

$$\delta T = T - T_a$$

Equations (31) and (32) are functions of ρ_4 . By evaluating these equations at $\rho_4 = \rho_a$, approximate values of H_4 and P_4 result. Substituting these approximate values (H_s and P_s) into the left-hand side of Eqs. (38) and (39), and combining so that δT is eliminated, yields

$$\delta\rho = \frac{(H_s - H_a) \frac{\partial P}{\partial T} \Big|_a - (P_s - P_a) \frac{\partial H}{\partial T} \Big|_a}{\frac{\partial P}{\partial T} \Big|_a \frac{\partial H}{\partial \rho} \Big|_a - \frac{\partial P}{\partial \rho} \Big|_a \frac{\partial H}{\partial T} \Big|_a} \quad (40)$$

The partial derivatives are evaluated by the finite difference relations

$$\frac{\partial P}{\partial T} \Big|_a = \frac{P(T_a + \Delta T, \rho_a) - P(T_a, \rho_a)}{\Delta T}$$

$$\frac{\partial H}{\partial T} \Big|_a = \frac{H(T_a + \Delta T, \rho_a) - H(T_a, \rho_a)}{\Delta T}$$

$$\frac{\partial H}{\partial \rho} \Big|_a = \frac{H(T_a, \rho_a + \Delta\rho) - H(T_a, \rho_a)}{\Delta\rho}$$

$$\frac{\partial P}{\partial \rho} \Big|_a = \frac{P(T_a, \rho_a + \Delta\rho) - P(T_a, \rho_a)}{\Delta\rho}$$

where $\Delta\rho = 10^{-4}\rho$ and $\Delta T = 500^\circ\text{K}$. The value of ΔT is dictated by the temperature increment for which values of enthalpy and free energy are tabulated in the program library. The results obtained with the 500°K increment have been found to be very good.

Now, the value of $\delta\rho$ obtained from the evaluation of Eq. (40) yields a density $(\rho)_n = (\rho)_n + \delta\rho$ which is closer to the desired value ρ_4 . By reevaluating the quantities in the right-hand side of Eq. (40) at the new value of density, further improvements result. When

$$\frac{(\delta\rho)_n}{(\rho_4)_n} \leq 10^{-3},$$

the value of $(\rho_4)_{n+1}$ is considered to be a solution. Using this value for ρ_4 , the values of H_4 and P_4 are evaluated using Eqs. (31) and (32), and the value of T_4 is obtained from Eq. (38).

V. PROGRAM DESCRIPTION

The numerical solution procedures discussed earlier have been programmed in Fortran for use on the IBM 7090 computer so that the following combinations of problem cases can be considered:

1. The Mollier data case. In this case, the program calculates the chemical equilibrium properties and composition of a gaseous mixture of specified temperature, density, and initial composition. The computation takes about 2 sec per temperature-density point.
2. Moving normal shock case. In this case, the program calculates the properties of a moving shock when the temperature (T_2), initial temperature (T_1), pressure (P_1), and chemical composition are specified. The computer requires about 15 sec for each solution.
3. Combination normal shock case. In this case, the moving normal shock problem is first solved. Then the properties and velocities associated with the reflected and the standing shock are determined. The time required for this case is 30–40 sec per moving shock.

The gross features of the program are shown in Fig. 6. For a detailed description, the flow diagram and program listing in the Appendix should prove helpful.

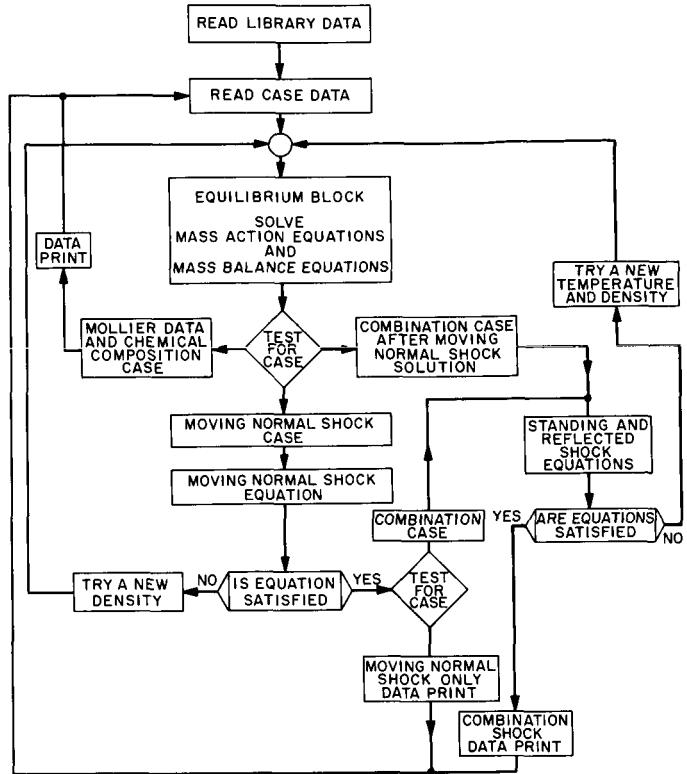


Fig. 6. Flow diagram for normal shock and chemical equilibrium program

VI. PROGRAM INPUT

The input data for the program is divided into two decks. The first deck, referred to as "library data," contains the thermochemical data for each chemical species considered to be a possible constituent of a planetary atmosphere. The entire library data deck is read into the machine following the program deck. The second deck of input data, referred to as "case data," is used to identify the particular case (i.e., Mollier data, moving normal shock, or combined normal shock), to specify which species of the library data constitute the mixture, and to specify certain initial and final state conditions. This division of the input data into two parts allows the thermochemistry data in the library to be used without rearrangement or modification, while making it accessible for modification if better values become available. The order of the program deck, library data deck, and case data decks is shown in Fig. 7.

A. Library Data

The library data deck is supplied with the program. It consists of approximately 600 IBM cards which contain the chemical formula, molecular weight, molal free energy, molal enthalpy, heat of formation, and other characteristic properties of 36 chemical species. The first 59 cards of the library data are shown in Table 1 and a list containing part of the library data for all species is shown in Table 2. Each of the species is assigned a library identification number which corresponds to the position of the thermochemistry data of that species in the library deck.

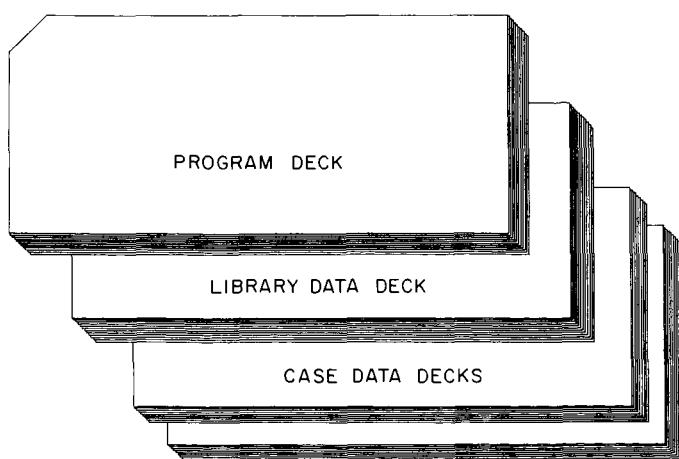


Fig. 7. Order of program and data decks

The order of the library data is as follows:

Card No. 1

The information on Card No. 1 is in format 2I2.* The first word on this card gives the number of chemical elements plus electrons which are listed in the library (in Table 1, this number is 05 since C, N, O, e⁻, A are present). The second word is the total number of species in the library (this number is 36).

Card No. 2

The information on this card is in format 1I2. This card supplies the number of temperatures for which thermochemistry data are tabulated (in the case of Table 1, the number is 39 because the temperatures range from 1000°K to 20,000°K in increments of 500°K).

Temperature Block

The temperature block of cards lists the values of temperature for which thermochemistry data are tabulated. The values range from 1000 to 20,000°K in increments of 500°K. The use of a temperature interval other than 500°K will require internal modification of the program. The format for a temperature block card is 20X, 5F7.1 (with a total of 39 values with 5 per card requires a block of 8 cards).

The remainder of the library data consists of thermochemistry data packets for each species which are arranged in the same order as the ID numbers in Table 2. Each packet contains the following cards:

Specie identification card. The first card of each packet contains, in the following order; the specie identification number (listed in Table 2); the chemical formula; the α_{ij} 's of the formula vector; and the molecular weight. The format for this card is 12X, A4, 6I2, 1F10.6.

Free energy block cards. Next in the packet is a block of cards which contain the values of $-(f^\circ - h_0^\circ)/T$ in cal/mole-°K for the temperatures listed in the temperature block. The number of values, the relative position in the sequence, and the number of cards should be

*Pertinent Fortran notation is given in the Appendix.

Table 1. Sample of library data

CN THERMOCHEMISTRY DATA PACKET	0536	39	1000.0 1500.0 2000.0 2500.0 3000.0 3500.0 4000.0 4500.0 5000.0 5500.0 6000.0 6500.0 7000.0 7500.0 8000.0 8500. 9000. 9500. 10000. 10500. 11000. 11500. 12000. 12500. 13000. 13500. 14000. 14500. 15000. 15500. 16000. 16500. 17000. 17500. 18000. 18500. 19000. 19500. 20000.	CARD No. 1 CARD No. 2
	1	CN 1 1 0 0 26.019000	TEMPERATURE BLOCK	
NO+ THERMOCHEMISTRY DATA PACKET	1	CN -(F-H*)/T 0.499797E 020.530001E 020.552316E 020.570236E 020.585367E 02 CN -(F-H*)/T 0.598565E 020.610328E 020.620966E 020.630685E 020.639630E 02 CN -(F-H*)/T 0.647913E 020.655620E 020.662822E 020.670000E 020.676500E 02 CN -(F-H*)/T 0.682739E 020.688489E 020.693954E 020.699162E 020.704136E 02 CN -(F-H*)/T 0.708895E 020.713457E 020.717836E 020.722046E 020.726098E 02 CN -(F-H*)/T 0.730003E 020.733770E 020.737408E 020.740924E 020.744325E 02 CN -(F-H*)/T 0.747616E 020.750805E 020.753896E 020.756893E 020.759802E 02 CN -(F-H*)/T 0.762627E 020.765371E 020.768038E 020.770631E 020.770631E 02 CN -(H-H*)/T 0.729132E 010.761998E 010.790163E 010.816956E 010.843572E 01 CN -(H-H*)/T 0.869227E 010.892772E 010.913472E 010.931099E 010.945791E 01 CN -(H-H*)/T 0.957870E 010.968000E 010.978000E 010.986500E 010.994500E 01 CN -(H-H*)/T 0.100180E 020.100843E 020.101321E 020.101749E 020.102130E 02 CN -(H-H*)/T 0.102468E 020.102763E 020.103017E 020.103230E 020.103404E 02 CN -(H-H*)/T 0.103538E 020.103634E 020.103692E 020.103714E 020.103702E 02 CN -(H-H*)/T 0.103656E 020.103578E 020.103471E 020.103337E 020.103177E 02 CN -(H-H*)/T 0.102994E 020.102789E 020.102564E 020.102322E 020.102322E 02 CN HEAT FORMATION 0.109000E 03	FREE ENERGY BLOCK	
	2	NO+ 0 1 1-1 0 30.008000		ENTHALPY BLOCK
CO THERMOCHEMISTRY DATA PACKET	2	NO--(F-H*)/T 0.488839E 020.518608E 020.540527E 020.558014E 020.572606E 02 NO--(F-H*)/T 0.585145E 020.596147E 020.605953E 020.614803E 020.622870E 02 NO--(F-H*)/T 0.630285E 020.637153E 020.643553E 020.649553E 020.655209E 02 NO--(F-H*)/T 0.660567E 020.665667E 020.670541E 020.675220E 020.679990E 02 NO--(F-H*)/T 0.684100E 020.688600E 020.692510E 020.697786E 020.701736E 02 NO--(F-H*)/T 0.705604E 020.709400E 020.713128E 020.716793E 020.720398E 02 NO--(F-H*)/T 0.723949E 020.727439E 020.730879E 020.734265E 020.737599E 02 NO--(F-H*)/T 0.740880E 020.744110E 020.747289E 020.750415E 020.750415E 02 NO+(H-H*)/T 0.720056E 010.749812E 010.774206E 010.792974E 010.807553E 01 NO+(H-H*)/T 0.819147E 010.828602E 010.836514E 010.843335E 010.849437E 01 NO+(H-H*)/T 0.855154E 010.860794E 010.866644E 010.872961E 010.879968E 01 NO+(H-H*)/T 0.887850E 010.896749E 010.906758E 010.917927E 010.928500E 01 NO+(H-H*)/T 0.941000E 010.960000E 010.980999E 010.998099E 010.101593E 02 NO+(H-H*)/T 0.103434E 020.105302E 020.107176E 020.109038E 020.110869E 02 NO+(H-H*)/T 0.112654E 020.114378E 020.116030E 020.117600E 020.119080E 02 NO+(H-H*)/T 0.120466E 020.121755E 020.122943E 020.124032E 020.124032E 02 NO+ HEAT FORMATION .234800E03	HEAT OF FORMATION	
	3	CO 1 0 1 0 0 28.011000		
	CO -(F-H*)/T 0.487737E 020.517779E 020.539915E 020.557564E 020.572279E 02 CO -(F-H*)/T 0.584915E 020.595994E 020.605863E 020.614765E 020.622873E 02 CO -(F-H*)/T 0.630321E 020.637210E 020.643621E 020.649621E 020.655242E 02 CO -(F-H*)/T 0.660591E 020.665648E 020.670466E 020.675075E 020.679900E 02 CO -(F-H*)/T 0.683800E 020.688000E 020.692232E 020.696171E 020.700021E 02 CO -(F-H*)/T 0.703793E 020.707479E 020.711141E 020.714731E 020.718271E 02 CO -(F-H*)/T 0.721766E 020.725216E 020.728624E 020.731989E 020.735314E 02 CO -(F-H*)/T 0.738596E 020.741835E 020.745032E 020.748184E 020.748184E 02 CO (H-H*)/T 0.725783E 010.757231E 010.781677E 010.800020E 010.814077E 01 CO (H-H*)/T 0.825165E 010.834156E 010.841626E 010.847973E 010.853491E 01 CO (H-H*)/T 0.858416E 010.862967E 010.867355E 010.871801E 010.876532E 01 CO (H-H*)/T 0.881779E 010.887768E 010.894709E 010.902786E 010.912147E 01			

identical to the temperature block cards. The format for a free energy block card is 20X, 5E12.6.

Enthalpy block cards. Each packet contains a block of cards with the values of $(h^\circ - h_0^\circ)/T$ in cal/mole-°K for the temperatures listed in the temperature block. The sequence and format are the same as in the free energy block.

Energy of formation card. The last card of each packet contains the value of the heat of formation, h° , in kcal/mole for the species associated with the packet. The format of this card is 20X, 1E12.6.

The thermochemistry data packet for the compound CN, which is the first packet in the library data deck, is

Table 2. Library thermochemistry data

ID No. <i>i</i>	FORMULA	FORMULA VECTOR $\alpha_{i,32} \alpha_{i,33} \alpha_{i,34} \alpha_{i,35} \alpha_{i,36}$					Molecular weight	Heat of formation, kcal/mole
		1	1	0	0	0		
1	CN	1	1	0	0	0	26.019	109.0
2	NO ⁺	0	1	1	-1	0	30.008	234.8
3	CO	1	0	1	0	0	28.011	-27.202
4	NO	0	1	1	0	0	30.008	-21.477
5	NO ₂	0	1	2	0	0	46.008	8.766
6	N ₂ O	0	2	1	0	0	44.016	20.309
7	CO ₂	1	0	2	0	0	44.011	-93.9643
8	N ₂	0	2	0	0	0	28.016	0
9	O ₂	0	0	2	0	0	32.000	0
10	C ⁺⁺	1	0	0	-3	0	12.0094	2095.69
11	C ⁺	1	0	0	-2	0	12.0099	991.689
12	C ⁺	1	0	0	-1	0	12.0105	429.537
13	C ⁻	1	0	0	1	0	12.0115	141.0
14	CO ₊	1	0	1	-1	0	28.011	295.977
15	C ₂ N ₂	2	2	0	0	0	52.038	73.4
16	C ₂	2	0	0	0	0	24.022	196.3
17	C ₃	3	0	0	0	0	36.003	188.0
18	N ⁺⁺⁺	0	1	0	-3	0	14.0064	2224.25
19	N ⁺⁺	0	1	0	-2	0	14.0069	1130.22
20	N ⁺	0	1	0	-1	0	14.0075	447.564
21	N ₂ ⁺	0	2	0	-1	0	28.016	359.306
22	O ⁺⁺⁺	0	0	1	-3	0	15.9984	2449.47
23	O ⁺⁺	0	0	1	-2	0	15.9989	1182.60
24	O ⁺	0	0	1	-1	0	15.9995	372.942
25	O ⁻	0	0	1	1	0	16.00055	25.1935
26	O ₂ ⁻	0	0	2	1	0	32.000	-23.00
27	O ₂ ⁺	0	0	2	-1	0	32.000	277.918
28	O ₃	0	0	3	0	0	48.000	34.639
29	A ⁺⁺⁺	0	0	0	-3	1	39.9423	1943.49
30	A ⁺⁺	0	0	0	-2	1	39.9428	1000.28
31	A ⁺	0	0	0	-1	1	39.9434	363.345
32	C	1	0	0	0	0	12.0110	169.99
33	N	0	1	0	0	0	14.008	112.507
34	O	0	0	1	0	0	16.000	58.9725
35	e	0	0	0	1	0	0.000549	0
36	A	0	0	0	0	1	39.944	0

shown in Table 1. The last card of the library data deck should be a heat of formation card for argon.

The values for the thermochemistry library data supplied with the program were taken from the following sources:

- For the atomic species A, A⁺, A⁺⁺, N, N⁺, N⁺⁺, O⁺, O⁺⁺, O⁺⁺⁺, C, C⁺, C⁺⁺, C⁺⁺⁺, O⁻, and e⁻, the data was taken from Browne (Ref. 8).
- For the linear polyatomic molecules CO₂ and N₂O, the values in the temperature range between 1000 and 10,000°K were taken from Browne (Ref. 9). For

the range from 10,000 to 20,000°K, the specific heat was assumed to be constant and equal to the value at 10,000°K. Under these conditions, the values are given by

$$\frac{h^\circ - h_0^\circ}{T} = (C_P)_{10,0000^\circ\text{K}} + \left[\left(\frac{h^\circ - h_0^\circ}{T} \right)_{10,0000^\circ\text{K}} - (C_P)_{10,0000^\circ\text{K}} \right] \frac{10,000}{T} \quad (41)$$

$$-\left(\frac{f^\circ - h_0^\circ}{T} \right) = -\left(\frac{f^\circ - h_0^\circ}{T} \right)_{10,0000^\circ\text{K}} + \left(\frac{h^\circ - h_0^\circ}{T} \right)_{10,0000^\circ\text{K}} - (C_P)_{10,0000^\circ\text{K}} + (C_P)_{10,0000^\circ\text{K}} \times \ln \left(\frac{T}{10,000} \right) + \left[(C_P)_{10,0000^\circ\text{K}} - \left(\frac{h^\circ - h_0^\circ}{T} \right)_{10,0000^\circ\text{K}} \right] \frac{10,000}{T} \quad (42)$$

where $10,000^\circ\text{K} \leq T \leq 20,000^\circ\text{K}$

- For the nonlinear molecular species NO₂ and O₃, the values in the low temperature range, 1000 to 10,000°K, were taken from Ref. 10. The high temperature values were obtained by the constant specific heat procedure described above.
- For the diatomic molecular species O₂, N₂, NO, CO, O₂⁺, N₂⁺, NO⁺, CO⁺, and O₂⁻ values were taken from Ref. 11.
- For the species CN, C₂, C⁻, C₃, and C₂N₂, the values were taken from Ref. 12, except for the high temperature range where the values for C₃ and C₂N₂ were calculated using Eqs. (41) and (42).
- For the ion A⁺⁺, values were taken from Ref. 13.

The values used seem to be the best for the temperature range considered because of the assumptions made in the calculation of the partition functions and the agreement with other published thermochemistry values.

B. Case Data

The case data deck communicates to the computer both control data and thermodynamic condition data. The control data are used to inform the computer as to which "problem case" is to be considered and when "new data" are to be read into the machine. The "new data" may be either a change of initial pressure, initial temperature, initial mole fraction composition, or a complete change of the problem case and initial mixture

constituents. Proper use of the control data will allow the user to run any combination of problem cases while varying the initial thermodynamic state and chemical composition at will.

The arrangement of the case data cards is summarized in Fig. 8. The format for the case data deck will be illustrated by the three following examples.

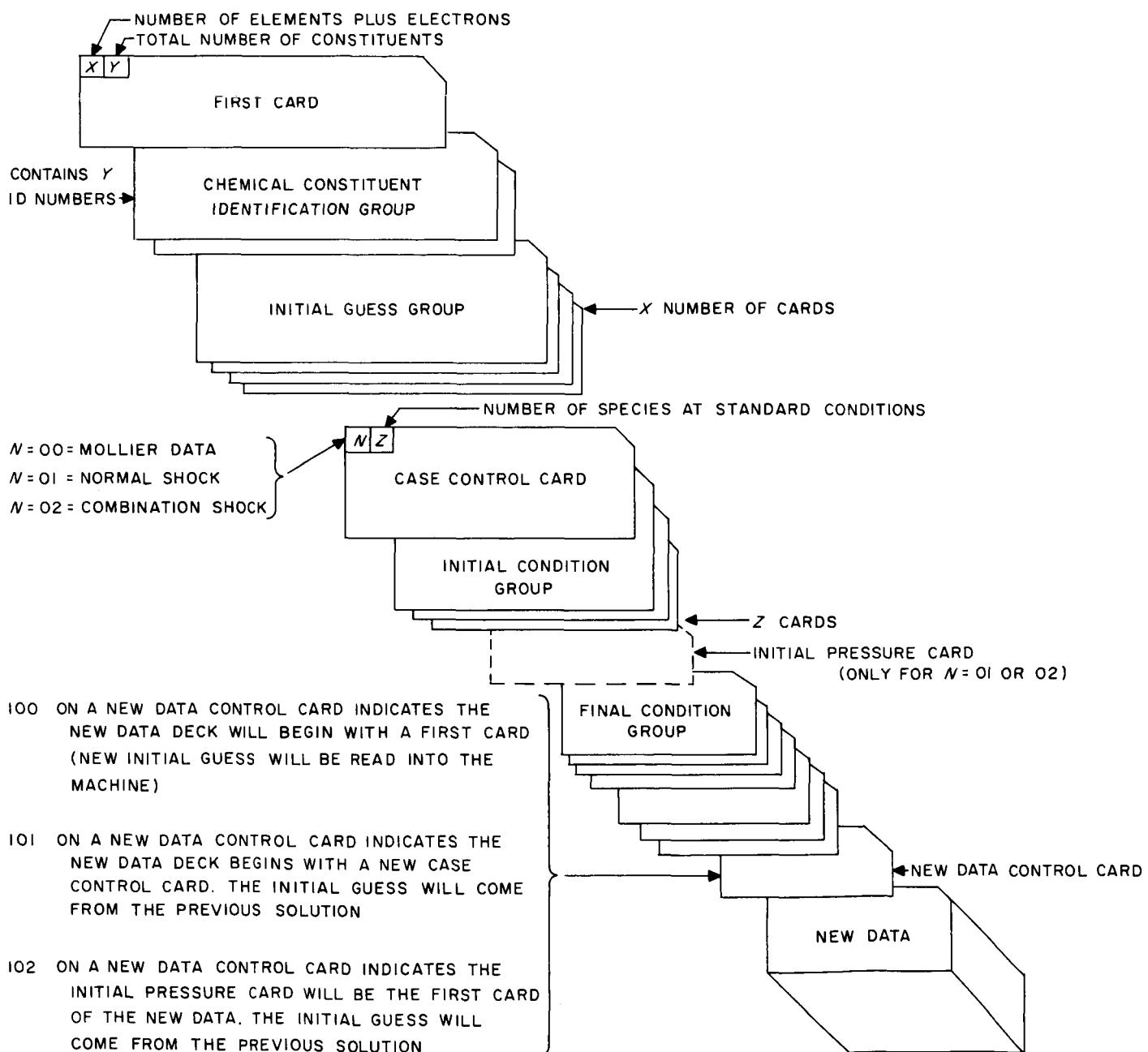


Fig. 8. The case data deck

Example 1. Determine the thermodynamic properties for densities (ρ/ρ_A) of 0.1 and 0.01 and temperatures between 3000 and 7000°K. The symbol ρ_A is the density of air at standard conditions.

Example 2. Determine the thermodynamic properties and velocities associated with a normal shock in an initial mixture composed of 30% CO₂ and 70% N₂. The initial temperature is 300°K, and the initial pressure is 0.004 atm. The temperatures in the shock-heated gas are 4500°K, 5000°K, 5500°K, and 6000°K. Also, at the same final temperatures as listed above, consider the properties of shocks in a mixture of 50% CO₂ and 50% N₂, with an initial temperature of 300°K and an initial pressure of 0.004 atm.

Example 3. Determine the properties of both reflected and standing shocks resulting from traveling incident shocks in an air-like mixture composed of 78.08% N₂, 20.95% O₂ and 0.97% A. The initial temperature of the gaseous mixture is 300°K. The initial

pressures considered are 0.001 and 0.01 atm. The temperatures behind the incident shock range from 4000 to 8000°K.

The form of case data for these examples is given in Tables 3, 4, and 5. The explanation of the format of the cards follows.

First Card

The first card of the case data deck supplies the total number of chemical species (compounds, ions, atoms, and the electron) and the total number of chemical elements (including the electron as a chemical element) which comprise the high temperature chemical equilibrium mixture. The information on this card is in format 2I2. The first word is the total number of elements in the mixture. The second word is the total number of chemical species.

In Example 1, the possible constituents of the high temperature mixture are N₂, N⁺⁺, N⁺, N₂⁺, N, and e⁻. The seven chemical species are composed of chemical elements N and e⁻. Thus, the first word is 02, and the second is 07.

Table 3. Example 1: Mollier data case

	10	20	30	40	50	60	70	80
0207								
N	8	18	19	20	21	33	35	
E-	0	600000E-07						
	0	100000E-13						
0001								
8 N2	1	00000	208698E+04	3000000E+03				
05	1	00000E	00					
06	1	00000E	00					
07	1	00000E	00					
08	1	00000E	00					
09	1	00000E	00					
10	1	00000E	00					
11	1	00000E	00					
12	1	00000E	00					
13	1	00000E	00					
13	1	000000E	-01					
12	1	000000E	-01					
11	1	000000E	-01					
10	1	000000E	-01					
09	1	000000E	-01					
08	1	000000E	-01					
07	1	000000E	-01					
06	1	000000E	-01					
05	1	000000E	-01					

Table 4. Example 2: Moving normal shock case (30% CO₂ — 70% N₂ and 50% CO₂ — 50% N₂)

4	3	2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
C	2	1	2	2	2	3	2	4	2	5	2	6	2	7	2	8	3	2	9	3	2	10	
N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
E-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
I	2																						
7	C	0	2	.3	0	0	0	-	.9	1	7	0	6	7	E	+0	5	.3	0	0	0	0	
8	N	2	0	.7	0	0	0	.	.2	0	8	6	9	8	E	+0	4	.3	0	0	0	0	
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
I	1																						
I	0																						
I	9																						
I	8																						
I	0	1																					
A	1	0	2																				
7	C	0	2	.5	0	0	0	-	.9	1	7	0	6	7	E	+0	5	.3	0	0	0	0	
8	N	2	0	.5	0	0	0	.	.2	0	8	6	9	8	E	+0	4	.3	0	0	0	0	
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
I	1																						
I	0	2	0	3	0	4	0	5	0	6	0	7	0	8	0	9	0	10	0	11	0	12	
I	13	0	14	0	15	0	16	0	17	0	18	0	19	0	20	0	21	0	22	0	23	0	24
I	25	0	26	0	27	0	28	0	29	0	30	0	31	0	32	0	33	0	34	0	35	0	36
I	37	0	38	0	39	0	40	0	41	0	42	0	43	0	44	0	45	0	46	0	47	0	48
I	49	0	50	0	51	0	52	0	53	0	54	0	55	0	56	0	57	0	58	0	59	0	60
I	61	0	62	0	63	0	64	0	65	0	66	0	67	0	68	0	69	0	70	0	71	0	72
I	73	0	74	0	75	0	76	0	77	0	78	0	79	0	80	0	81	0	82	0	83	0	84
I	85	0	86	0	87	0	88	0	89	0	90	0	91	0	92	0	93	0	94	0	95	0	96
I	97	0	98	0	99	0	100	0	101	0	102	0	103	0	104	0	105	0	106	0	107	0	108
I	109	0	110	0	111	0	112	0	113	0	114	0	115	0	116	0	117	0	118	0	119	0	120
I	121	0	122	0	123	0	124	0	125	0	126	0	127	0	128	0	129	0	130	0	131	0	132
I	133	0	134	0	135	0	136	0	137	0	138	0	139	0	140	0	141	0	142	0	143	0	144
I	145	0	146	0	147	0	148	0	149	0	150	0	151	0	152	0	153	0	154	0	155	0	156
I	157	0	158	0	159	0	160	0	161	0	162	0	163	0	164	0	165	0	166	0	167	0	168
I	169	0	170	0	171	0	172	0	173	0	174	0	175	0	176	0	177	0	178	0	179	0	180
I	181	0	182	0	183	0	184	0	185	0	186	0	187	0	188	0	189	0	190	0	191	0	192
I	193	0	194	0	195	0	196	0	197	0	198	0	199	0	200	0	201	0	202	0	203	0	204
I	205	0	206	0	207	0	208	0	209	0	210	0	211	0	212	0	213	0	214	0	215	0	216
I	217	0	218	0	219	0	220	0	221	0	222	0	223	0	224	0	225	0	226	0	227	0	228
I	229	0	230	0	231	0	232	0	233	0	234	0	235	0	236	0	237	0	238	0	239	0	240
I	241	0	242	0	243	0	244	0	245	0	246	0	247	0	248	0	249	0	250	0	251	0	252
I	253	0	254	0	255	0	256	0	257	0	258	0	259	0	260	0	261	0	262	0	263	0	264
I	265	0	266	0	267	0	268	0	269	0	270	0	271	0	272	0	273	0	274	0	275	0	276
I	277	0	278	0	279	0	280	0	281	0	282	0	283	0	284	0	285	0	286	0	287	0	288
I	289	0	290	0	291	0	292	0	293	0	294	0	295	0	296	0	297	0	298	0	299	0	300
I	301	0	302	0	303	0	304	0	305	0	306	0	307	0	308	0	309	0	310	0	311	0	312
I	313	0	314	0	315	0	316	0	317	0	318	0	319	0	320	0	321	0	322	0	323	0	324
I	325	0	326	0	327	0	328	0	329	0	330	0	331	0	332	0	333	0	334	0	335	0	336
I	337	0	338	0	339	0	340	0	341	0	342	0	343	0	344	0	345	0	346	0	347	0	348
I	349	0	350	0	351	0	352	0	353	0	354	0	355	0	356	0	357	0	358	0	359	0	360
I	361	0	362	0	363	0	364	0	365	0	366	0	367	0	368	0	369	0	370	0	371	0	372
I	373	0	374	0	375	0	376	0	377	0	378	0	379	0	380	0	381	0	382	0	383	0	384
I	385	0	386	0	387	0	388	0	389	0	390	0	391	0	392	0	393	0	394	0	395	0	396
I	397	0	398	0	399	0	400	0	401	0	402	0	403	0	404	0	405	0	406	0	407	0	408
I	409	0	410	0	411	0	412	0	413	0	414	0	415	0	416	0	417	0	418	0	419	0	420
I	421	0	422	0	423	0	424	0	425	0	426	0	427	0	428	0	429	0	430	0	431	0	432

Table 5. Example 3: Combination normal shock case (air mixture)

4	2	4	5	6	8	9	18	19	20	21	22	23	24	25	26	27	28	29	30	31	
3	3	34	35	36																	
N	0	1	80000E-05																		
0	0	1	60000E-03																		
E-	0	0	300000E-08																		
A	0	0	420000E-05																		
0	2	0	3	0	4	0	5	0	6	0	7	0	8	0	9	0	10	0	11	0	
I	12	0	13	0	14	0	15	0	16	0	17	0	18	0	19	0	20	0	21	0	22
I	23	0	24	0	25	0	26	0	27	0	28	0	29	0	30	0	31	0	32	0	33
I	34	0	35	0	36	0	37	0	38	0	39	0	40	0	41	0	42	0	43	0	44
I	45	0	46	0	47	0	48	0	49	0	50	0	51	0	52	0	53	0	54	0	55
I	56	0	57	0	58	0	59	0	60	0	61	0	62	0	63	0	64	0	65	0	66
I	67	0	68	0	69	0	70	0	71	0	72	0	73	0	74	0	75	0	76	0	77
I	78	0	79	0	80	0	81	0	82	0	83	0	84	0	85	0	86	0	87	0	88
I	89	0	90	0	91	0	92	0	93	0	94	0	95	0	96	0	97	0	98	0	99
I	100	0	101	0	102	0	103	0	104	0	105										

In Example 2, the chemical species are all those combinations of C, N, O, and e^- which are listed in Table 2. There are 32 of these. The number of elements plus electrons is 04.

In Example 3, the constituent species are the combinations of N, O, e^- , and A which are listed in Table 2. There are 24 species which contain these four chemical elements.

Chemical Constituent Identification Group

This group consists of up to two cards which list the identification numbers of the constituent chemical species of the high temperature mixture. The identification numbers are found in Table 2. Each number is listed with an I4 format. With this format, there are a maximum of 20 identification numbers on each card. The identification numbers should be in order so that the chemical elements occur in the last positions. The number of identification numbers must equal the number in the second word position of the "first card."

For Example 1, the 7 constituents N_2 , N^{++} , N^{++} , N^+ , N_2^+ , N, and e^- have the identification numbers 8, 18, 19, 20, 21, 33, and 35, respectively. The seven values can be listed on one card. Two cards are required to list the 32 constituent identification numbers for Example 2 and two are required for identification numbers for Example 3.

Initial Guess Cards

There is an initial concentration guess card for each chemical element in the mixture. The number of initial guess cards is equal to the number appearing in the first word position of the "first card." The format for an initial guess card is 4X, 1E12.6. The first word position contains the chemical symbol for the element. The second word position contains the approximate concentration (mole/l) of the element at the first equilibrium state for which a solution is sought. The order of the initial guess cards should be the same as the order of the elements in Table 2.

As the convergence of numerical procedure for the chemical equilibrium computation is dependent upon the knowledge of a set of concentrations which nearly satisfy the mass action and mass balance equations, the initial guess values are very important. If the initial guess values are in error by more than an order of magnitude, the convergence of the chemical equilibrium calculation is doubtful. The procedure for selecting the initial guesses

is somewhat of an art which develops with the use of the program.

The program automatically uses the concentrations from the previous equilibrium calculation as the initial guess values for the next chemical equilibrium computation. Thus, the set of final and initial condition states should be arranged in an orderly progression to insure convergence of the numerical procedure.

In the case of Example 1, the concentrations of 6.0×10^{-8} mole/l for N and 1×10^{-14} mole/l for the electrons are the approximate concentrations at a temperature of $3000^\circ K$ and a density of 0.129 g/l. For example 2, the concentrations (in mole/l) of

C	1.76×10^{-5}
N	3.85×10^{-4}
O	6.44×10^{-4}
e^-	4.74×10^{-7}

are associated with the temperature of $6000^\circ K$ and the density of about 0.05 g/l. For Example 3, the concentrations of

N	1.8×10^{-6}
O	1.6×10^{-4}
e^-	3.0×10^{-9}
A	4.2×10^{-6}

are for a temperature of $4000^\circ K$ and a density of about 0.01 g/l.

Case Control Card

The case control card contains two numbers in I2 format. The first number identifies the case of the problem to be considered. If this number is 00, the indication is that Mollier data is to be generated. If this number is 01, moving normal shock problems are to be solved. The number 02 indicates combination shock problems. No other values are valid for the first word position on the case control card.

The second number on the card identifies the number of compounds present in the mixture at standard conditions. This number must equal the number of cards in the initial condition group.

Initial Condition Group

The format for the initial condition control card is I2, A4, 1F7.5, 2E12.6. There is one card for each of the initial constituents of the mixture. The number of cards in this group must be equal to the number in the second word position of the control card.

The first word is the species identification number taken from Table 1. The second word is the chemical symbol for the species. The third word is the mole-fraction of the species in the mixture at standard conditions. For the Mollier data case, this is all the information required on an initial condition group card, and any information in the fourth and fifth word positions is read into the computer but is not utilized in the computations.

For the moving and combination normal shock cases, the values in the fourth and fifth word positions are the initial partial molal enthalpy of the species in cal/mole and initial temperature, T_1 . The molal enthalpy can be found in Browne (Refs. 8, 9, 10, 11, 12, and 13).

The order of the cards within the initial condition group is not important; however, the best procedure would be to arrange the identification numbers which appear on them in order. The data on these cards are not only used to calculate the thermodynamic properties of the gas at standard and initial conditions, but also are used with the library data to calculate the values of B_i which appear in the mass action equations.

For Example 1, the 100% N₂-Mollier data case, there is only one card in the initial condition group. The first word is 08 (which agrees with the specie identification number for N₂ in Table 1). The position and format of the chemical formula and mole-fraction are shown in Table 3. Normally, the fourth and fifth word positions would be vacant for a Mollier data case. The values listed for the enthalpy and temperature will not effect the operation of the program as they are not used in Mollier data computations.

For Example 2, the first card of the initial condition group corresponds to CO₂ and contains the specie ID number of 07, the mole-fractional concentration at standard conditions of 0.3, the initial molal enthalpy of the compound—91706.7 cal/mole, and the initial temperature of 300°K. The second card corresponds to the compound N₂ and contains the ID number of 08, the mole-fraction of 0.7, the molal enthalpy of 2086.98 cal/mole, and the initial temperature of 300°K.

For Example 3, the cards list:

ID No.	Chemical symbol	Mole-fraction @ STP	Initial molal enthalpy, cal/mole	Initial temperature, °K
08	N ₂	0.7808	2086.98	300
09	O ₂	0.2095	2089.78	300
36	A	0.0097	1490.45	300

Initial Pressure Card

The initial pressure card is not included when the Mollier data case is to be run. The card contains the pressure of the gas in atmospheres before the passage of the shock. The pressure value is in a format E12.6.

In Example 1, the initial pressure card is not necessary.

In Example 2, the initial pressure is 0.04 atm. Farther down in the new case data, the initial pressure of 0.04 atm is repeated for the 50%-CO₂ and 50%-N₂ mixture.

In Example 3, the first initial pressure is 0.001 atm. In the new data, the initial pressure is changed to 0.01 atm.

Final Condition Group

The final condition group is composed of an unlimited number of cards. There is one card for each thermodynamic or shock condition. The thermodynamic condition associated with the first card of this group should be compatible with the concentrations listed on the initial guess cards.

For the Mollier data cases, each card specifies the temperature and density of the thermodynamic state for which the chemical equilibrium composition and properties are to be calculated. The format for a Mollier data case, final condition group card is 1I3, 1E12.6. The first word is the temperature ID number. The second word is the ratio of density at the solution point to density of air at standard conditions. Experience has shown that the most efficient way of calculating data over a range of temperatures and densities is to calculate a series of temperatures while holding the density constant, then change density by not over an order of magnitude and calculate through the series of temperatures in reverse order, and so on. The values of the temperature are limited to those in Table 6.

For the normal shock cases, the format of the final condition group cards is 1I3. Each card lists the temperature identification number from Table 6 which corre-

Table 6. Temperature identification number

Temperature ID No.	Temperature, °K	Temperature ID No.	Temperature, °K
1	1000	21	11,000
2	1500	22	11,500
3	2000	23	12,000
4	2500	24	12,500
5	3000	25	13,000
6	3500	26	13,500
7	4000	27	14,000
8	4500	28	14,500
9	5000	29	15,000
10	5500	30	15,500
11	6000	31	16,000
12	6500	32	16,500
13	7000	33	17,000
14	7500	34	17,500
15	8000	35	18,000
16	8500	36	18,500
17	9000	37	19,000
18	9500	38	19,500
19	10,000	39	20,000
20	10,500		

sponds to the temperature T_2 . The first card of a final condition group will use the concentrations listed on the initial guess cards.

New Data Control Card

A new data control card is used for the following options:

1. To change initial pressure in normal shock and combined shock cases.
2. To change initial mixture mole-fractions and/or to change initial enthalpy and temperature and/or change cases.

3. To completely change the problem by reading in a completely new deck of case data beginning with the "first card."

If the computations are complete when the last card of the final condition group has been processed, then the new data card is not used. However, if as shown in Table 5, an option such as (1) is considered, with the initial pressure changed from 10^{-3} to 10^{-2} atm, then a new data card with 102 must be used to preface the new data. In this option, the new data consists of a new pressure card followed by a new final condition group. Note that the last temperature and first temperature of the new data are the same to insure convergence at the new pressure.

If an option such as (2) is desired, the new data control card should contain a 101. This will cause the machine to read in a new set of data which should consist of new case control card, initial condition group, initial pressure card, and final condition group. An example illustrating the use of the 101 new data control card is given in Table 4, where the card is used to change the mole-fraction composition of the CO₂-N₂ mixture for a moving normal shock case. Because the program uses the concentrations from the previous calculation as the initial guesses for the new calculations, the change in initial state and concentration should not be large.

The option (3) is achieved by using a 100 new data control card. After this card, a completely new set of case data, beginning with "first card," should follow. A 100 new data control card used between each of the example data of Tables 3, 4, and 5 would allow the three problems to be solved in succession.

VII. PROGRAM OUTPUT

The output for the first solution of each of the three example cases are shown in Tables 7, 8, and 9.

For a Mollier data case, the format is shown in Table 7. Listed in the first row are the values of $\rho_0 = \rho_A$, which is the density of air in g/l at standard conditions, and the number of iterations through the mass action and mass balance equations. The chemical concentration of each specie in the mixture is listed next. The first two columns are the concentrations of the species in mole/l. The first column contains the values from the next to last iteration and the second column contains those from the last iteration. The third column lists the concentrations in the units of particles per cubic centimeter. The fourth column lists the mole-fraction concentration. The fifth column lists the negative of the natural logarithm of the equilibrium constant in terms of partial pressure and for formation of the species from the elements. The value K_P is equal to the value K_i defined in Eq. (8).

The tabulation of specie concentration is followed by a display of the thermodynamic properties in dimensionless form. These values are the temperature in °K; the dimensionless density; the pressure in atmospheres; Z as defined in Eq. (10); the total number of molecular weights in one liter of the high temperature gas; HM_0/RT_0 (the enthalpy per unit mass in dimensionless form); and SM_0/R (the entropy per unit mass in dimensionless form).

The R is the universal gas constant 1.98726 cal/mole-°K, M_0 is the "cold" molecular weight, T_0 is 273.15°K. The cold molecular weight and composition of the mixture at standard conditions are listed at the bottom of the display.

The forms of the output data for the moving normal shock case and the combination normal shock case are shown in Tables 8 and 9. The two are the same except for the listing on Table 9 of the properties of the standing normal shock and reflected normal shock at the bottom of the page. The number of iterations at the top of both tables refers to iterations through the moving normal shock equations. The description of the concentration and thermodynamic property display given above for the Mollier data case is applicable to both of the shock solution cases. The heading "Initial Conditions" is equivalent to subscripting the properties under that heading with 1 or ∞ . Similarly, the heading "Final Conditions" is equivalent to subscripting the properties with 2.

The quantities listed in the lower left-hand corner of the tables are shock velocity, U_s , or free flight velocity, U_F , in ft/sec; the dimensionless stagnation enthalpy on a free flight body; the pressure ratio P_2/P_1 or P_2/P_∞ for the moving shock; the density ratio ρ_2/ρ_1 , or ρ_2/ρ_∞ for the moving shock; the velocity, U_g , associated with the moving normal shock; and the "cold" molecular weight of the mixture.

Table 7. Chemical equilibrium composition and properties of a complex mixture

RHOO = 0.129233E 01 GM/L		NUMBER OF ITERATIONS = 3		
CONCENTRATION - MOLE/LITER		CONCENTRATION MOLE FRACTION -LOGE(KP)		
(FINAL-1)	(FINAL)	PARTICLES/CC		
N2	0.460987E-02	0.461281E-02	0.277847E 19	0.999987E 00 -0.223703E 02
N++	0.750000E-35	1.000000E-35	0.602338E-14	0.216785E-32 0.338254E 03
N++	0.750000E-35	1.000000E-35	0.602338E-14	0.216785E-32 0.158792E 03
N+	0.692379E-17	0.700843E-17	0.422145E 04	0.151932E-14 0.496502E 02
N2+	0.940388E-14	0.952177E-14	0.573533E 07	0.206418E-11 0.313144E 02
N	0.600577E-07	0.600768E-07	0.361866E 14	0.130237E-04 0.
E-	0.964652E-14	0.952877E-14	0.573954E 07	0.206569E-11 0.
FINAL CONDITIONS				
TEMP DEG K	RHU/RHOO	P/PU	Z	SUM CUN MOL/L
0.300000E 04	0.100000E-00	0.113556E 01	0.100001E 01	0.461287E-02
 HM0/RT0 SMO/R				
0.446348E 02	0.319581E 02			
 COLD MIXTURE MOLE WT. = 28.015999				
 TOTAL CONCENTRATION OF N2 AT STANDARD CONDITIONS 100.0000 PER CENT				

Table 8. Real gas normal shock wave solution

RHO0 = 0.129233E 01 GM/L	NUMBER OF ITERATIONS = 2				
TOTAL CONCENTRATION OF CO2 AT STANDARD CONDITIONS	30.0000 PER CENT				
TOTAL CONCENTRATION OF N2 AT STANDARD CONDITIONS	70.0000 PER CENT				
C CONCENTRATION - MOLE/LITER	CONCENTRATION PARTICLES/CC	MOLE FRACTION	-LOGE(KP)		
(FINAL-1)	(FINAL)				
CN 0.236157E-05	0.236156E-05	0.142246E 16	0.779588E-03	0.352009E-00	
NO+ 0.436598E-06	0.436596E-06	0.262979E 15	0.144127E-03	0.139684E 02	
CO 0.632193E-03	0.632190E-03	0.380792E 18	0.208695E-00	-0.471744E 01	
NO 0.193559E-04	0.193558E-04	0.116587E 17	0.638964E-02	0.185848E 01	
NO2 0.105952E-09	0.105951E-09	0.638182E 11	0.349759E-07	0.128368E 02	
N2O 0.107750E-08	0.107749E-08	0.649014E 12	0.355696E-06	0.999696E 01	
CO2 0.136121E-06	0.136120E-06	0.819900E 14	0.449351E-04	0.258875E 01	
N2 0.131756E-02	0.131756E-02	0.793614E 18	0.434945E-00	-0.288248E 01	
O2 0.531632E-06	0.531627E-06	0.320219E 15	0.175498E-03	0.597370E 01	
C++ 1.000000E-35	1.000000E-35	0.602338E-14	0.330115E-32	0.140504E 03	
C++ 0.125182E-21	0.125183E-21	0.754023E-01	0.413247E-19	0.561222E 02	
C+ 0.295379E-07	0.295380E-07	0.177919E 14	0.975095E-05	0.147093E 02	
C- 0.170487E-10	0.170486E-10	0.102690E 11	0.562800E-08	0.553019E 01	
CO+ 0.159146E-07	0.159146E-07	0.958598E 13	0.525365E-05	0.141905E 02	
C2N2 0.737596E-11	0.737591E-11	0.444279E 10	0.243490E-08	0.662363E 01	
C2 0.780018E-08	0.780018E-08	0.469834E 13	0.257495E-05	0.297522E 01	
C3 0.175422E-11	0.175422E-11	0.105663E 10	0.579094E-09	0.662773E 01	
N+++ 1.000000E-35	1.000000E-35	0.602338E-14	0.330115E-32	0.155974E 03	
N++ 0.265935E-26	0.265936E-26	0.160184E 05	0.877896E-24	0.699713E 02	
N+ 0.396389E-08	0.396390E-08	0.238761E 13	0.130854E-05	0.198074E 02	
N2+ 0.230612E-08	0.230612E-08	0.138906E 13	0.761284E-06	0.186915E 02	
O+++ 1.000000E-35	1.000000E-35	0.602338E-14	0.330115E-32	0.178400E 03	
O++ 0.420052E-30	0.420053E-30	0.253014E-09	0.138666E-27	0.792450E 02	
O+ 0.806348E-08	0.806347E-08	0.485693E 13	0.266187E-05	0.196177E 02	
O- 0.987135E-09	0.987127E-09	0.594584E 12	0.325865E-06	0.508160E 01	
O2- 0.100269E-11	0.100267E-11	0.603948E 09	0.330997E-09	0.108365E 02	
O2+ 0.271775E-09	0.271773E-09	0.163699E 12	0.897164E-07	0.218706E 02	
O3 0.133027E-12	0.133025E-12	0.801260E 08	0.439135E-10	0.200374E 02	
C 0.176189E-04	0.176189E-04	0.106125E 17	0.581625E-02	0.	
N 0.387105E-03	0.387104E-03	0.233168E 18	0.127789E-00	0.	
O 0.651394E-03	0.651391E-03	0.392357E 18	0.215034E-00	0.	
E- 0.495651E-06	0.495649E-06	0.298548E 15	0.163621E-03	0.	
INITIAL CONDITIONS					
TEMP DEG-K	RHD/RHO0	P/PO	HMO/RT0	SUM CON MOL/L	
0.300000E 03	0.412585E-02	0.400000E-02	-0.479922E 02	0.162488E-03	
FINAL CONDITIONS					
TEMP DEG-K	RHO/RHO0	P/PO	HMO/RT0	SUM CON MOL/L	
0.600000E 04	0.552157E-01	0.149143E 01	0.171447E 03	0.302925E-02	
SMO/R	Z				
0.464909E 02	0.139304E 01				
SHOCK VELOCITY-----	0.181337E 05FPS				
STAGNATION ENTHALPY---	0.172679E 03HMO/RT0				
P2/PI-----	0.372859E 03				
RHO2/RHO1-----	0.133829E 02				
VELOCITY BEHIND SHOCK-	0.167787E 05FPS				
COLD MIXTURE MOLE WT. =	32.814498				
0.362998E 04 0.363040E 04 -0.423187E-00					

Listed under the heading "Standing Normal Shock Relations" on Table 9 are: the dimensionless enthalpy, H_3M_0/RT_0 ; the density, ρ_3/ρ_A ; the temperature, T_3 ; the pressure, P_3 , in atmospheres; the dimensionless stagnation enthalpy on the model; the velocity, U_3 , in ft/sec; the pressure ratio P_3/P_2 ; and the density ratio, ρ_3/ρ_2 . The standing shock solution does not give model stagnation conditions but the equilibrium state of the gas at position 3 has been found to be very close to the state at the stagnation point.

Under the heading "Reflected Shock Relations" are listed: the dimensionless enthalpy, H_4M_0/RT_0 ; the den-

sity, ρ_4/ρ_A ; the temperature, T_4 ; the pressure, P_4 , in atmospheres; the pressure ratio, P_4/P_2 ; the density ratio, ρ_4/ρ_2 ; and the reflected shock velocity in ft/sec.

The program prints one shock solution per page. The three values at the bottom of Table 8 indicate how well the Hugoniot equation is satisfied. The first two numbers are the values of the left and right sides of Eq. (20). The third is the difference between them.

In addition to the above "scheduled" output, the program has been designed to halt all computation when the

Table 9. Real gas normal shock wave solution

RHOO = 0.129233E 01 GM/L		NUMBER OF ITERATIONS = 2	
TOTAL CONCENTRATION OF N2 AT STANDARD CONDITIONS		78.0800 PER CENT	
TOTAL CONCENTRATION OF O2 AT STANDARD CONDITIONS		20.9500 PER CENT	
TOTAL CONCENTRATION OF A AT STANDARD CONDITIONS		0.9700 PER CENT	
CONCENTRATION - MOLE/LITER	CONCENTRATION PARTICLES/CC	MOLE FRACTION	-LOGE(KP)
(FINAL-1)	(FINAL)		
N0+	0.303156E-08	0.303155E-08	0.182602E 13
NO	0.112343E-04	0.112342E-04	0.676681E 16
N02	0.243465E-09	0.243462E-09	0.146647E 12
N20	0.226633E-09	0.226631E-09	0.136508E 12
N2	0.335974E-03	0.335972E-03	0.202369E 18
O2	0.403715E-05	0.403711E-05	0.243171E 16
N++	1.000000E-35	1.000000E-35	0.602338E-14
N++	1.000000E-35	1.000000E-35	0.602338E-14
N+	0.129406E-14	0.129406E-14	0.779463E 06
N2+	0.126121E-13	0.126121E-13	0.759672E 07
O+++	1.000000E-35	1.000000E-35	0.602338E-14
O++	1.000000E-35	1.000000E-35	0.602338E-14
O+	0.353606E-12	0.353606E-12	0.212990E 09
O-	0.117383E-10	0.117382E-10	0.707038E 10
O2-	0.202903E-12	0.202901E-12	0.122215E 09
O2+	0.172218E-11	0.172217E-11	0.103733E 10
O3	0.567736E-12	0.567728E-12	0.341964E 09
A+++	1.000000E-35	1.000000E-35	0.602338E-14
A++	1.000000E-35	1.000000E-35	0.602338E-14
A+	0.209036E-15	0.209036E-15	0.125910E 06
N	0.178844E-05	0.178843E-05	0.107724E 16
O	0.164476E-03	0.164475E-03	0.990698E 17
E-	0.302171E-08	0.302170E-08	0.182008E 13
A	0.425477E-05	0.425475E-05	0.256280E 16
INITIAL CONDITIONS			
TEMP DEG-K	RHO/RHOO	P/PO	HMO/RT0
0.300000E 03	0.910503E-03	1.000000E-03	0.383512E 01
SUM CON MOL/L			
FINAL CONDITIONS			
TEMP DEG-K	RHO/RHOO	P/PO	HMO/RT0
0.400000E 04	0.983154E-02	0.171260E-00	0.105982E 03
SMO/R	Z		
0.399649E 02	0.118953E 01		
SHOCK VELOCITY-----0.1319E 05FPS		STANDING NORMAL SHOCK RELATIONS	
STAGNATION ENTHALPY---0.1069E 03HMO/RT0		REFLECTED SHOCK RELATIONS	
P2/P1-----	0.1713E 03	ENTHALPY-----	0.1879E 03HMO/RT0
RHO2/RHO1-----	0.1080E 02	RHO3/RHOO-----	0.5275E-01
VELOCITY BEHIND SHOCK-0.1197E 05FPS		TEMPERATURE DEG-K---	0.6065E 04
COLD MIXTURE MOLE WT--0.2897E 02		P3/PO-----	0.1529E 01
		STAGNATION ENTHALPY--0.1908E 03HMO/RT0	P4/P2-----0.1245E 02
		VELOCITY BEHIND SHOCK-0.2231E 04FPS	RHO4/RHO2-----0.6697E 01
		P3/P2-----	REFLECTED VELOCITY--0.2101E 04
		RHO3/RHO2-----	0.5365E 01

number of iteration loops through the equilibrium block exceeds 50, or through the moving normal shock equations exceeds 20. After 50 equilibrium block iterations, the program prints "equilibrium state not reached in

50 iterations" followed by a tabulation of the concentrations for the last two iterations. After 20 normal shock iterations, the machine prints "no Hugoniot solution in 20 iterations" and halts.

NOMENCLATURE

B_i	concentration of the i th element at STP, moles/l.	P_i	partial pressure of the i th specie.
C_i	quantity defined in Eq. (35).	R	universal gas constant, 1.98726 cal/mole-°K.
$C_{P,i}$	molal specific heat at constant pressure for the i th specie, cal/mole-°K.	S	entropy per unit mass.
$C_{V,i}$	molal specific heat at constant volume for the i th specie, cal/mole-°K.	T	Temperature, °K.
D_i	constant defined with Eqs. (33) and (34).	U	velocity.
f_i°	partial molal free energy of the i th specie evaluated at a pressure of one atmosphere, cal/mole.	v	= $1/\rho$ specific volume of gas, l/g
H	enthalpy per unit mass.	$X^{(j)}$	the chemical symbol for the j th numbered chemical element.
h_i°	partial molal enthalpy of the i th specie evaluated at a pressure of one atmosphere, cal/mole.	$Y^{(i)}$	the chemical symbol for the i th numbered compound.
h_{0i}°	energy of formation for one mole of the i th specie at a pressure of one atmosphere and a temperature of 0°K, cal/mole.	Y_{ij}	matrix coefficient defined in Eq. (35).
K	thermal conductivity.	Z	$= \frac{M_0}{M}$
K_i	equilibrium constant for the i th compound (Eq. 8).	a_{ij}	the number of atoms of the j th numbered element in the molecule of the i th numbered specie.
M_0	molecular weight at standard conditions (cold molecular weight).	η	Viscosity.
N_i	number of moles of the i th constituent.	μ_i	Chemical potential of the i th specie.
n_i	concentration of the i th specie, mole/l.	ρ	mass density.
P	total pressure of mixture.	ρ_0	density of mixture at STP.
		() _A	property of air at STP.
		() ₀	property of mixture at STP.

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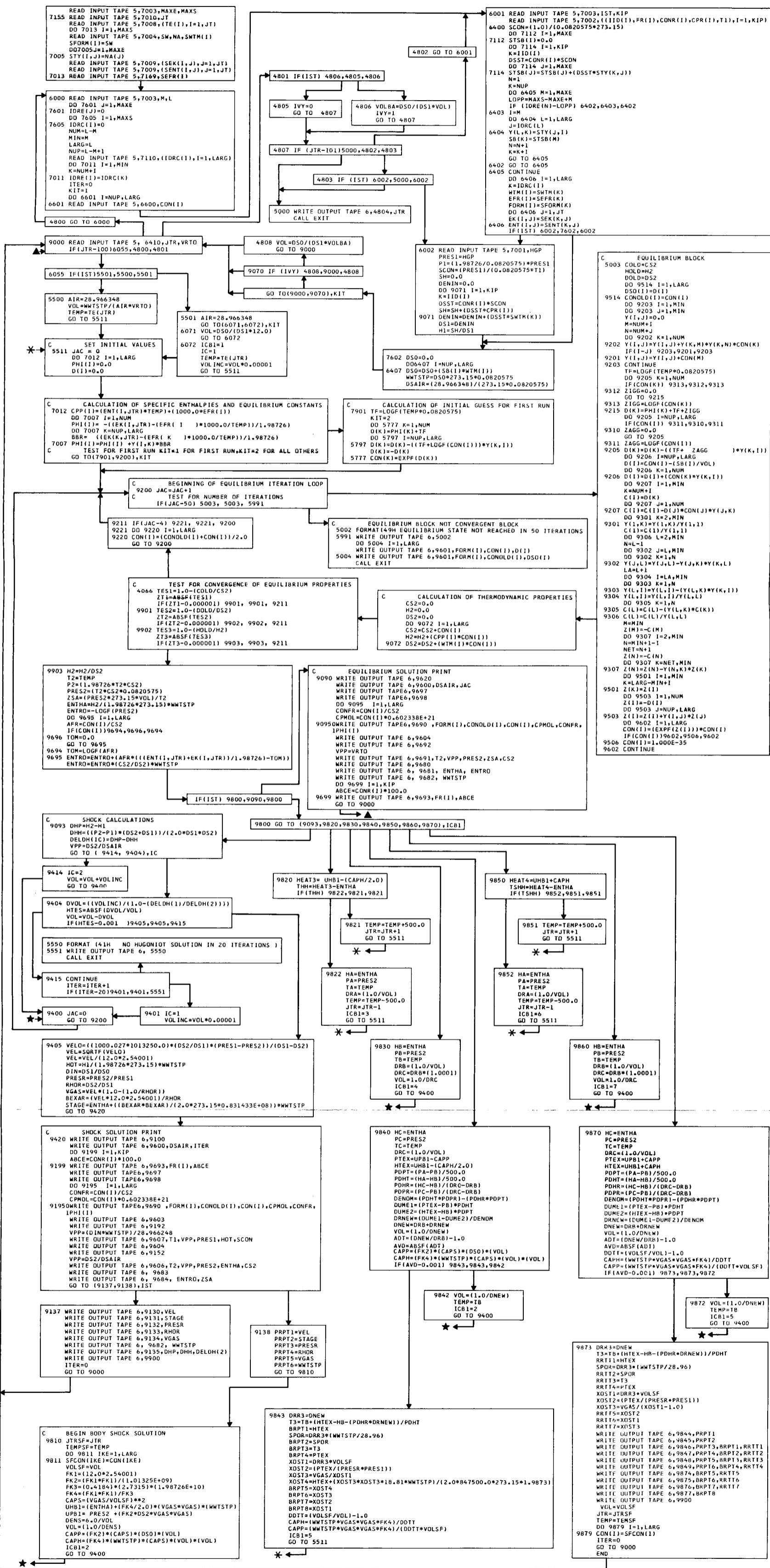
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APPENDIX

Flow Diagram and Description of Thermochemistry and Normal Shock Computer Program



KEY TO FORMAT STATEMENTS

I-format is used to enter fixed point numbers. The prefix numeral indicates the number of words. The suffix numeral indicates the number of spaces per word. For example, 2I3 is used to enter the numbers 5 and 416 in the following key punch form:

Word No. 1 Word No. 2

0	0	5		4	1	6
---	---	---	--	---	---	---

F-format is used to enter floating point numbers for which the exponent notation is not needed to locate the decimal position. The prefix indicates the number of words. The suffix, which is a decimal, indicates the number of spaces per word and the number of digits from the right to the decimal position. For example, 3F5.3 is used to enter the numbers 0.72, 4.95 and 0.012 in the following key punch form:

Word No. 1 Word No. 2 Word No. 3

0	.	7	2	0		4	.	9	5	0		0	.	0	1	2
---	---	---	---	---	--	---	---	---	---	---	--	---	---	---	---	---

E-format is used to enter floating point numbers for which the exponent notation is used to locate the decimal position. The prefix indicates the number of words. The suffix, which is a decimal number, indicates the number of spaces per word and the number of digits following the decimal. For example, 2E12.6 is used to enter the numbers 6.32×10^6 and .072 in the following key punch form:

Word No. 1

0	.	6	3	2	0	0	0	E	+	0	6	0	.	7	2	0	0	0	0	E	-	0	1
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

A-format is used to enter alpha-numeric data. The suffix is used to indicate the number of spaces per word. For example, A4 is used to enter CO₂ in the following key punch form:

	C	0	2
--	---	---	---

X-format is used for spacing. No values are read or printed.

Blanks in the key punch fields are read as zeros.

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ODIMENSION NA(6),WTM(36),SB(36),Y(36,36),PHI(36),CON(36),D(36),
1CPP(36),CONR(36),WTR(36),CPR(36),CONOLD(36),FORM(36),C(39),Z(36),
2TE(39),FR(36),ENT(36,39),EK(36,39),DSO(36),DELDH(2),EFR(36,39),
3SFCON(36),CONC(36),CONB(36),CONA(36),SFORM(36),STY(36,6),STS(6),
4SEK(36,39),SENT(36,39),SEFR(36),IDRC(36),IDRE(6),IID(36),SWTM(36)
4804 FORMAT(15H THE VALUE JTR=,I4,2X,I2THIS NOT VALID)
6410 FORMAT(1I3,1E12.6)
6501 FORMAT(12,A4,1F7.5)
6600 FORMAT(4X,1E12.6)
6602 FORMAT(1E12.6)
7001 FORMAT(1E12.6)
7002 FORMAT(12,A4,1F7.5,2E12.6)
7003 FORMAT(2I2)
7004 FORMAT(12X,A4,6I2,1F10.6)
7008 FORMAT(20X,5F7.1)
7009 FORMAT(20X,5E12.6)
7010 FORMAT(1I2)
7110 FORMAT(20I4)
7169 FORMAT(20X,1E12.6)
9192 FORMAT(7X, 91H TEMP DEG-K      RHO/RH00      P/P0      HMO/RT0
    1 SUM CON MOL/L )
9607 FORMAT(6X,5E14.6/ )
9152 FORMAT(7X, 91H TEMP DEG-K      RHO/RH00      P/P0      HMO/RT0
    1 SUM CON MOL/L )
9606 FORMAT(6X,7E14.6 /)
9683 FORMAT(7X, 20HSMO/R      Z      )
9684 FORMAT(6X, 2E14.6//)
9130 FORMAT(3X,22HSHOCK VELOCITY----- 1E14.6, 5HFPS )
9131 FORMAT(3X,22HSTAGNATION ENTHALPY--- 1E14.6, 7HHMO/RT0)
9132 FORMAT(3X,22HP2/P1----- 1E14.6 )
9133 FORMAT(3X,22HRHO2/RHO1----- 1E14.6 )
9134 FORMAT(3X,22HVELOCITY BEHIND SHOCK- 1E14.6, 5HFPS )
9900 FORMAT(1H1)
9135 FORMAT(1H0 3E14.6)
9600 FORMAT(9H   RH00 =1E14.6,5H GM/L 7X,22HNUMBER OF ITERATIONS =112)
9601 FORMAT(3X,A4,2X,2E12.6)
9603 FORMAT(22H INITIAL CONDITIONS )
9604 FORMAT(20H FINAL CONDITIONS )
9608 FORMAT(23H CONCENTRATION-M/L D      )
9610 FORMAT(19H SHOCK VELOCITY =1E12.6      )
9690 FORMAT(3X,A4,2X,5E14.6)
96970FORMAT(10X,70HCONCENTRATION - MOLE/LITER CONCENTRATION MOLE FRAC
    ITION -LOGE(KP)      )
9698 FORMAT(11X,40HFINAL-1)      (FINAL)      PARTICLES/CC      )
9692 FORMAT(7X, 70H TEMP DEG*K      RHO/RH00      P/P0      Z
    1 SUM CON MOL/L )
9680 FORMAT(10X,19H HMO/RT0      SMO/R)
9691 FORMAT(6X,5E14.6///)
9681 FORMAT(6X,2E14.6///)
9682 FORMAT(26H COLD MIXTURE MOLE WI. =F10.6///)
9693 FORMAT(3X,23HTOTAL CONCENTRATION OF A4,23HAT STANDARD CONDITIONS
    1 F8.4 ,12H PER CENT      )
9620 FORMAT(1H1 9X,70H CHEMICAL EQUILIBRIUM COMPOSITION AND PROPERTIES
    OF A COMPLEX MIXTURE //)
9100 FORMAT(1H1 9X,38H REAL GAS NORMAL SHOCK WAVE SOLUTION // )

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READ INPUT TAPE 5,7003,MAXE,MAXS
7155 READ INPUT TAPE 5,7010,JT
READ INPUT TAPE 5,7008,(TE(I),I=1,JT)
DO 7013 I=1,MAXS
READ INPUT TAPE 5,7004,SW,NA,SWTM(I)
SFORM(I)=SW
DO 7005 J=1,MAXE
7005 STY(I,J)=NA(J)
READ INPUT TAPE 5,7009,(SEK(I,J),J=1,JT)
READ INPUT TAPE 5,7009,(SENT(I,J),J=1,JT)
7013 READ INPUT TAPE 5,7169,SEFR(I)
6000 READ INPUT TAPE 5,7003,M,L
DO 7601 J=1,MAXE
7601 IDRE(J)=0
DO 7605 I=1,MAXS
7605 IDRC(I)=0
NUM=L-M
MIN=M
LARG=L
NUP=L-M+1
READ INPUT TAPE 5,7110,(IDRC(I),I=1,LARG)
DO 7011 I=1,MIN
K=NUM+I
7011 IDRE(I)=IDRC(K)
ITER=0
KIT=1
DO 6601 I=NUP,LARG
6601 READ INPUT TAPE 5,6600,CON(I)
6001 READ INPUT TAPE 5,7003,IST,KIP
READ INPUT TAPE 5,7002,((IID(I),FR(I),CONR(I),CPR(I),T1),I=1,KIP)
6400 SCON=(1.0)/(0.0820575*273.15)
DO 7112 I=1,MAXE
7112 STSB(I)=0.0
DO 7114 I=1,KIP
K=IID(I)
DSST=CONR(I)*SCON
DO 7114 J=1,MAXE
7114 STSB(J)=STSB(J)+(DSST*STY(K,J))
N=1
K=NUP
DO 6405 M=1,MAXE
LOPP=MAXS-MAXE+M
IF (IDRE(N)-LOPP) 6402,6403,6402
6403 I=M
DO 6404 L=1,LARG
J=IDRC(L)
6404 Y(L,K)=STY(J,I)
SB(K)=STSB(M)
N=N+1
K=K+1
GO TO 6405
6402 GO TO 6405
6405 CONTINUE
DO 6406 I=1,LARG
K=IDRC(I)
WTM(I)=SWTM(K)

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EFR(I)=SEFR(K)
FORM(I)=SFORM(K)
DO 6406 J=1,JT
EK(I,J)=SEK(K,J)
6406 ENT(I,J)=SENT(K,J)
IF(IST) 6002,7602,6002
6002 READ INPUT TAPE 5,7001,HGP
PRES1=HGP
P1=(1.98726/0.0820575)*PRES1
SCUN=(PRES1)/(0.0820575*T1)
SH=0.0
DENIN=0.0
DO 9071 I=1,KIP
K=IID(I)
DSST=CONR(I)*SCON
SH=SH+(DSST*CPR(I))
9071 DENIN=DENIN+(DSST*SWTM(K))
DS1=DENIN
H1=SH/DS1
7602 DSO=0.0
DO6407 I=NUP,LARG
6407 DSO=DSO+(SB(I)*WTM(I))
WWTSTP=DSO*273.15*0.0820575
DSAIR=(28.966348)/(273.15*0.0820575)
GO TO(9000,9070),KIT
9070 IF (IVY) 4808,9000,4808
4808 VOL=DSO/(DS1*VOLBA)
GO TO 9000
9000 READ INPUT TAPE 5, 6410,JTR,VRTU
IF(JTR-100)6055,4800,4801
4800 GO TO 6000
4801 IF(IST) 4806,4805,4806
4805 IVY=0
GO TO 4807
4806 VOLBA=DSO/(DS1*VOL)
IVY=1
GO TO 4807
4807 IF (JTR-101)5000,4802,4803
4802 GO TO 6001
4803 IF (IST) 6002,5000,6002
5000 WRITE OUTPUT TAPE 6,4804,JTR
CALL EXIT
6055 IF(IST)5501,5500,5501
5500 AIR=28.966348
VOL=WWTSTP/(AIR*VRTU)
TEMP=TE(JTR)
GO TO 5511
5501 AIR=28.966348
GO TO(6071,6072),KIT
6071 VOL=DSO/(DS1*12.0)
GO TO 6072
6072 ICBI=1
IC=1
TEMP=TE(JTR)
VOLINC=VOL*0.00001
GO TO 5511

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C      SET INITIAL VALUES
5511 JAC = 0
      DO 7012 I=1,LARG
      PHI(I)=0.0
      D(I)=0.0
C      CALCULATION OF SPECIFIC ENTHALPIES AND EQUILIBRIUM CONSTANTS
7012 CPP(I)=(ENT(I,JTR)*TEMP)+(1000.0*EFR(I))
      DO 7007 I=1,NUM
      PHI(I)= -((EK(I,JTR)-(EFR( I     )*1000.0/TEMP))/1.98726)
      DO 7007 K=NUP,LARG
      BBR= ((EK(K,JTR)-(EFR( K     )*1000.0/TEMP))/1.98726)
7007 PHI(I)=PHI(I) +Y(I,K)*BBR
C      TEST FOR FIRST RUN KIT=1 FOR FIRST RUN, KIT=2 FOR ALL OTHERS
      GO TO(7901,9200),KIT
C      CALCULATION OF INITIAL GUESS FOR FIRST RUN
7901 TF=LOGF(TEMP*0.0820575)
      KIT=2
      DO 5777 K=1,NUM
      D(K)=PHI(K)+TF
      DO 5797 I=NUP,LARG
5797 D(K)=D(K)-((TF+LOGF(CON(I)))*Y(K,I))
      D(K)=-D(K)
5777 CON(K)=EXP(F(D(K)))
C      BEGINNING OF EQUILIBRIUM ITERATION LOOP
9200 JAC=JAC+1
C      TEST FOR NUMBER OF ITERATIONS
      IF(JAC-50) 5003, 5003, 5991
C      EQUILIBRIUM BLOCK NOT CONVERGENT BLOCK
5002 FORMAT(49H EQUILIBRIUM STATE NOT REACHED IN 50 ITERATIONS
5991 WRITE OUTPUT TAPE 6,5002
      DO 5004 I=1,LARG
      WRITE OUTPUT TAPE 6,9601,FORM(I),CON(I),D(I)
5004 WRITE OUTPUT TAPE 6,9601,FORM(I),CONOLD(I),DSO(I)
      CALL EXIT
C      EQUILIBRIUM BLOCK
5003 COLD=CS2
      HOLD=H2
      DOLD=DS2
      DO 9514 I=1,LARG
      DSO(I)=D(I)
9514 CONOLD(I)=CON(I)
      DO 9203 I=1,MIN
      DO 9203 J=1,MIN
      Y(I,J)=0.0
      M=NUM+I
      N=NUM+J
      DO 9202 K=1,NUM
9202 Y(I,J)=Y(I,J)+Y(K,M)*Y(K,N)*CON(K)
      IF(I-J) 9203,9201,9203
9201 Y(I,J)=Y(I,J)+CON(M)
9203 CONTINUE
      TF=LOGF(TEMP*0.0820575)
      DO 9205 K=1,NUM
      IF(CON(K)) 9313,9312,9313
9312 ZIGG=0.0
      GO TO 9215

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9313 ZIGG=LOGF(CON(K))
9215 D(K)=PHI(K)+TF+ZIGG
      DO 9205 I=NUP,LARG
      IF(CON(I)) 9311,9310,9311
9310 ZAGG=0.0
      GO TO 9205
9311 ZAGG=LOGF(CON(I))
9205 D(K)=D(K)-((TF+    ZAGG      )*Y(K,I))
      DO 9206 I=NUP,LARG
      D(I)=CON(I)-(SB(I)/VOL)
      DO 9206 K=1,NUM
9206 D(I)=D(I)+(CON(K)*Y(K,I))
      DO 9207 I=1,MIN
      K=NUM+I
      C(I)=D(K)
      DO 9207 J=1,NUM
9207 C(I)=C(I)-D(J)*CON(J)*Y(J,K)
      DO 9301 K=2,MIN
9301 Y(1,K)=Y(1,K)/Y(1,1)
      C(1)=C(1)/Y(1,1)
      DO 9306 L=2,MIN
      N=L-1
      DO 9302 J=L,MIN
      DO 9302 K=1,N
9302 Y(J,L)=Y(J,L)-Y(J,K)*Y(K,L)
      LA=L+1
      DO 9304 I=LA,MIN
      DO 9303 K=1,N
9303 Y(L,I)=Y(L,I)-(Y(L,K)*Y(K,I))
9304 Y(L,I)=Y(L,I)/Y(L,L)
      DO 9305 K=1,N
9305 C(L)=C(L)-(Y(L,K)*C(K))
9306 C(L)=C(L)/Y(L,L)
      M=MIN
      Z(M)=-C(M)
      DO 9307 I=2,MIN
      N=MIN+1-I
      NET=N+1
      Z(N)=-C(N)
      DO 9307 K=NET,MIN
9307 Z(N)=Z(N)-Y(N,K)*Z(K)
      DO 9501 I=1,MIN
      K=LARG-MIN+I
9501 Z(K)=Z(I)
      DO 9503 I=1,NUM
      Z(I)=-D(I)
      DO 9503 J=NUP,LARG
9503 Z(I)=Z(I)+Y(I,J)*Z(J)
      DO 9602 I=1,LARG
      CON(I)=(EXP(Z(I)))*CON(I)
      IF(CON(I))9602,9506,9602
9506 CON(I)=1.000E-35
9602 CONTINUE
C      CALCULATION OF THERMODYNAMIC PROPERTIES
      CS2=0.0
      H2=0.0

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DS2=0.0
DO 9072 I=1,LARG
CS2=CS2+CON(I)
H2=H2+(CPP(I)*CON(I))
9072 DS2=DS2+(WTM(I)*CON(I))
C      TEST FOR CONVERGENCE OF EQUILIBRIUM PROPERTIES
4066 TES1=1.0-(COLD/CS2)
ZT1=ABSF(TES1)
IF(ZT1-0.000001) 9901, 9901, 9211
9901 TES2=1.0-(DOLD/DS2)
ZT2=ABSF(TES2)
IF(ZT2-0.000001) 9902, 9902, 9211
9902 TES3=1.0-(HOLD/H2)
ZT3=ABSF(TES3)
IF(ZT3-0.000001) 9903, 9903, 9211
9211 IF(JAC-4) 9221, 9221, 9200
9221 DO 9220 I=1,LARG
9220 CON(I)=(CONOLD(I)+CON(I))/2.0
GO TO 9200
9903 H2=H2/DS2
T2=TEMP
P2=(1.98726*T2*CS2)
PRES2=(T2*CS2*0.0820575)
ZSA=(PRES2*273.15*VOL)/T2
ENTHA=H2/(1.98726*273.15)*WWTSTP
ENTRO=-LOGF(PRES2)
DO 9695 I=1,LARG
AFR=CON(I)/CS2
IF(CON(I))9694,9696,9694
9696 TOM=0.0
GO TO 9695
9694 TOM=LOGF(AFR)
9695 ENTRO=ENTRO+(AFR*(((ENT(I,JTR)+EK(I,JTR))/1.98726)-TOM))
ENTRO=ENTRO*(CS2/DS2)*WWTSTP
IF(IST) 9800,9090,9800
9800 GO TO (9093,9820,9830,9840,9850,9860,9870),ICB1
C      SHOCK CALCULATIONS
9093 DHP=H2-M1
DHH=((P2-P1)*(DS2+DS1))/(2.0*DS1*DS2)
DELDH(IC)=DHP-DHH
VPP=DS2/DSAIR
GO TO ( 9414, 9404),IC
9414 IC=2
VOL=VOL+VOLINC
GO TO 9400
9401 IC=1
VOLINC=VOL*0.00001
9400 JAC=0
GO TO 9200
9404 DVOL=((VOLINC)/(1.0-(DELDH(1)/DELDH(2))))
HTES=ABSF(DVOL/VOL)
VOL=VOL-DVOL
IF(HTES-0.001) 9405,9405,9415
9415 CONTINUE
ITER=ITER+1
IF(ITER-20)9401,9401,5551

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5550 FORMAT (41H NO HUGONIOT SOLUTION IN 20 ITERATIONS )
5551 WRITE OUTPUT TAPE 6, 5550
      CALL EXIT
9405 VEL0=((1000.027*1013250.0)*(DS2/DS1)*(PRES1-PRES2))/(DS1-DS2)
      VEL=SQRTF(VEL0)
      VEL=VEL/(12.0*2.54001)
      HOT=H1/(1.98726*273.15)*WWTSTP
      DIN=DS1/DS0
      PRESR=PRES2/PRES1
      RHOR=DS2/DS1
      VGAS=VEL*(1.0-(1.0/RHOR))
      BEXAR=(VEL*12.0*2.54001)/RHOR
      STAGE=ENTHA+((BEXAR*BEXAR)/(2.0*273.15*0.831433E+08))*WWTSTP
      GO TO 9420
C      SHOCK SOLUTION PRINT
9420 WRITE OUTPUT TAPE 6,9100
      WRITE OUTPUT TAPE 6,9600,DSAIR,ITER
      DO 9199 I=1,KIP
      ABCE=CONR(I)*100.0
9199 WRITE OUTPUT TAPE 6,9693,FR(I),ABCE
      WRITE OUTPUT TAPE 6,9697
      WRITE OUTPUT TAPE 6,9698
      DO 9195 I=1,LARG
      CONFR=CON(I)/CS2
      CPMOL=CON(I)*0.602338E+21
91950 WRITE OUTPUT TAPE 6,9690 ,FORM(I),CONOLD(I),CON(I),CPMOL,CONFR,
      1PHI(I)
      WRITE OUTPUT TAPE 6,9603
      WRITE OUTPUT TAPE 6,9192
      VPP=(DIN*WWTSTP)/28.966248
      WRITE OUTPUT TAPE 6,9607,T1,VPP,PRES1,HOT,SCON
      WRITE OUTPUT TAPE 6,9604
      WRITE OUTPUT TAPE 6,9152
      VPP=DS2/DSAIR
      WRITE OUTPUT TAPE 6,9606,T2,VPP,PRES2,ENTHA,CS2
      WRITE OUTPUT TAPE 6, 9683
      WRITE OUTPUT TAPE 6, 9684, ENTRO,ZSA
      GO TO (9137,9138),IST
9138 PRPT1=VEL
      PRPT2=STAGE
      PRPT3=PRESR
      PRPT4=RHOR
      PRPT5=VGAS
      PRPT6=WWTSTP
      GO TO 9810
9137 WRITE OUTPUT TAPE 6,9130,VEL
      WRITE OUTPUT TAPE 6,9131,STAGE
      WRITE OUTPUT TAPE 6,9132,PRESR
      WRITE OUTPUT TAPE 6,9133,RHOR
      WRITE OUTPUT TAPE 6,9134,VGAS
      WRITE OUTPUT TAPE 6, 9682, WWTSTP
      WRITE OUTPUT TAPE 6,9135,DHP,DHH,DELDH(2)
      WRITE OUTPUT TAPE 6,9900
      ITER=0
      GO TO 9000
C      EQUILIBRIUM SOLUTION PRINT
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9090 WRITE OUTPUT TAPE 6,9620
      WRITE OUTPUT TAPE 6,9600,DSAIR,JAC
      WRITE OUTPUT TAPE6,9697
      WRITE OUTPUT TAPE6,9698
      DO 9095 I=1,LARG
      CONFR=CON(I)/CS2
      CPMOL=CON(I)*0.602338E+21
90950 WRITE OUTPUT TAPE6,9690 ,FORM(I),CONOLD(I),CON(I),CPMOL,CONFR,
      IPHI(I)
      WRITE OUTPUT TAPE 6,9604
      WRITE OUTPUT TAPE 6,9692
      VPP=VRTO
      WRITE OUTPUT TAPE 6,9691,T2,VPP,PRES2,ZSA,CS2
      WRITE OUTPUT TAPE 6,9680
      WRITE OUTPUT TAPE 6, 9681, ENTHA, ENTRO
      WRITE OUTPUT TAPE 6, 9682, WWTSTP
      DO 9699 I=1,KIP
      ABCE=CONR(I)*100.0
9699 WRITE OUTPUT TAPE 6,9693,FR(I),ABCE
      GO TO 9000
C      BEGIN BODY SHOCK SOLUTION
9810 JTRSF=JTR
      TEMPSF=TEMP
      DO 9811 IKE=1,LARG
9811 SFCON(IKE)=CON(IKE)
      VOLSF=VOL
      FK1=(12.0*2.54001)
      FK2=(FK1*FK1)/(1.01325E+09)
      FK3=(0.4184)*(2.7315)*(1.98726E+10)
      FK4=(FK1*FK1)/FK3
      CAPS=(VGAS/VOLSF)**2
      UHBL=(ENTHA)+(FK4/2.0)*(VGAS*VGAS)*(WWTSTP)
      UPBL= PRES2 +(FK2*DS2*VGAS*VGAS)
      DENS=6.0/VOL
      VOL=(1.0/DENS)
      CAPP=(FK2)*(CAPS)*(DS0)*(VOL)
      CAPH=(FK4)*(WWTSTP)*(CAPS)*(VOL)*(VOL)
      ICB1=2
      GO TO 9400
9820 HEAT3= UHBL-(CAPH/2.0)
      THH=HEAT3-ENTHA
      IF(THH) 9822,9821,9821
9821 TEMP=TEMP+500.0
      JTR=JTR+1
      GO TO 5511
9822 HA=ENTHA
      PA=PRES2
      TA=TEMP
      DRA=(1.0/VOL)
      TEMP=TEMP-500.0
      JTR=JTR-1
      ICB1=3
      GO TO 5511
9830 HB=ENTHA
      PB=PRES2
      TB=TEMP

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DR8=(1.0/VOL)
DRC=DR8*(1.0001)
VOL=1.0/DRC
ICB1=4
GO TO 9400
9840 HC=ENTHA
PC=PRES2
TC=TEMP
DRC=(1.0/VOL)
PTEX=UPB1-CAPP
HTEX=UHB1-(CAPH/2.0)
PDPT=(PA-PB)/500.0
PDHT=(HA-HB)/500.0
PDHR=(HC-HB)/(DRC-DRB)
PDPR=(PC-PB)/(DRC-DRB)
DENOM=(PDHT*PDPR)-(PDHR*PDPT)
DUME1=(PTEX-PB)*PDHT
DUME2=(HTEX-HB)*PDPT
DRNEW=(DUME1-DUME2)/DENOM
DNEW=DR8+DRNEW
VOL=(1.0/DNEW)
ADT=(DNEW/DRB)-1.0
AVU=ABSF(ADT)
CAPP=(FK2)*(CAPS)*(DSO)*(VOL)
CAPH=(FK4)*(WWTSTP)*(CAPS)*(VOL)*(VOL)
IF(AVD-0.001) 9843,9843,9842
9842 VOL=(1.0/DNEW)
TEMP=TB
ICB1=2
GO TO 9400
9843 DRR3=DNEW
T3=TB+(HTEX-HB-(PDHR*DRNEW))/PDHT
BRPT1=HTEX
SPOR=DRR3*(WWTSTP/28.96)
BRPT2=SPOR
BRPT3=T3
BRPT4=PTEX
XOST1=DRR3*VOLSF
XOST2=(PTEX/(PRESR*PRES1))
XOST3=VGAS/XOST1
XOST4=HTEX+(XOST3*XOST3*18.81*WWTSTP)/(2.0*847500.0*273.15*1.9873)
BRPT5=XUST4
BRPT6=XOST3
BRPT7=XOST2
BRPT8=XOST1
DDTT=(VOLSF/VOL)-1.0
CAPH=(WWTSTP*VGAS*VGAS*FK4)/DDTT
CAPP=(WWTSTP*VGAS*VGAS*FK4)/(DDTT*VOLSF)
ICB1=5
GO TO 5511
9850 HEAT4=UHB1+CAPH
TSHH=HEAT4-ENTHA
IF(TSHH) 9852,9851,9851
9851 TEMP=TEMP+500.0
JTR=JTR+1
GO TO 5511

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9852 HA=ENTHA
PA=PRES2
TA=TEMP
DRA=(1.0/VOL)
TEMP=TEMP-500.0
JTR=JTR-1
ICB1=6
GO TO 5511
9860 HB=ENTHA
PB=PRES2
TB=TEMP
DRB=(1.0/VOL)
DRC=DRB*(1.0001)
VOL=1.0/DRC
ICB1=7
GO TO 9400
9870 HC=ENTHA
PC=PRES2
TC=TEMP
DRC=(1.0/VOL)
PTEX=UPBL+CAPP
HTEX=UHBL+CAPH
PDPT=(PA-PB)/500.0
PDHT=(HA-HB)/500.0
PDHR=(HC-HB)/(DRC-DRB)
PDPR=(PC-PB)/(DRC-DRB)
DENOM=(PDHT*PDPR)-(PDHR*PDPT)
DUME1=(PTEX-PB)*PDHT
DUME2=(HTEX-HB)*PDPT
DRNEW=(DUME1-DUME2)/DENOM
DNEW=DRB+DRNEW
VOL=(1.0/DNEW)
ADT=(DNEW/DRB)-1.0
AVD=ABSF(ADT)
DDTT=(VOLSF/VOL)-1.0
CAPH=(WWTSTP*VGAS*VGAS*FK4)/DDTT
CAPP=(WWTSTP*VGAS*VGAS*FK4)/(DDT1*VOLSF)
IF(AVD-0.001) 9873,9873,9872
9872 VOL=(1.0/DNEW)
TEMP=TB
ICB1=5
GO TO 9400
9873 DRR3=DNEW
T3=TB+(HTEX-HB-(PDHR*DRNEW))/PDHT
RRTT1=HTEX
SPOR=DRR3*(WWTSTP/28.96)
RRTT2=SPOR
RRTT3=T3
RRTT4=PTEX
XOST1=DRR3*VOLSF
XOST2=(PTEX/(PRESR*PRES1))
XOST3=VGAS/(XOST1-1.0)
RRTT5=XUST2
RRTT6=XUST1
RRTT7=XOST3
9844 FORMAT(1X,22HSHOCK VELOCITY-----,1E10.4,7HFPS ,80H STANDING

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INORMAL SHOCK RELATIONS REFLECTED SHOCK RELATIONS
2)
9845 FORMAT(1X,22HSTAGNATION ENTHALPY---,1E10.4,7HHMO/RTO)
9846 FORMAT(1X,22HP2/P1-----,1E10.4,8X,22HENTHALPY-----
3----,1E10.4,8HHMO/RTO ,20HENTHALPY-----,1E10.4,7HHMO/RTO)
9847 FURMAT(1X,22HRHU2/RHO1-----,1E10.4,8X,22HRHO3/RHO0-----
1----,1E10.4,8X,20HRHU4/RHO0-----,1E10.4)
9848 FORMAT(1X,22HVELOCITY BEHIND SHOCK-,1E10.4,8HFPS ,22HTEMPERATU
2KE DEG-K----,1E10.4,8X,20HTEMPERATURE DEG-K---,1E10.4)
9849 FURMAT(1X,22HCOLD MIXTURE MOLE WT--,1E10.4,8X,22HP3/PO-----
1----,1E10.4,8X,20HP4/PO-----,1E10.4)
9874 FORMAT(41X,22HSTAGNATION ENTHALPY---,1E10.4,8HHMO/RTO ,20HP4/P2---
1-----,1E10.4)
9875 FORMAT(41X,22HVELOCITY BEHIND SHOCK-,1E10.4,8HFPS ,20HRHO4/RHO
12----,1E10.4)
9876 FORMAT(41X,22HP3/P2-----,1E10.4,8X,20HREFLECTED VELOC
ITY--,1E10.4)
9877 FORMAT(41X,22HRHU3/RHO2-----,1E10.4)
WRITE OUTPUT TAPE 6,9844,PRPT1
WRITE OUTPUT TAPE 6,9845,PRPT2
WRITE OUTPUT TAPE 6,9846,PRPT3,BRPT1,RRTT1
WRITE OUTPUT TAPE 6,9847,PRPT4,BRPT2,RRTT2
WRITE OUTPUT TAPE 6,9848,PRPT5,BRPT3,RRTT3
WRITE OUTPUT TAPE 6,9849,PRPT6,BRPT4,RRTT4
WRITE OUTPUT TAPE 6,9874,BRPT5,RRTT5
WRITE OUTPUT TAPE 6,9875,BRPT6,RRTT6
WRITE OUTPUT TAPE 6,9876,BRPT7,RRTT7
WRITE OUTPUT TAPE 6,9877,BRPT8
WRITE OUTPUT TAPE 6,9900
VUL=VOLSF
JTR=JTRSF
TEMP=TEMSE
DO 9879 I=1,LARG
9879 CON(I)=SFCON(I)
ITER=0
GO TO 9000
END(1,0,0,0,0,0,1,0,0,1,0,0,0,0,0,0)